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Micro- and macro-block factorizations for
regularized saddle point systems

by

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Micro- and macro-block factorizations for regularized saddle point systems

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Abstract

We present unique and existing micro-block and induced macro-block Crout-based factorizations for matrices from regularized saddle-point problems with semi-positive definite regularization block. For the classical case of saddle-point problems we show that the induced macro-block factorizations mostly reduces to the factorization presented in [24]. The presented factorization can be used as a direct solution algorithm for regularized saddle-point problems as well as it can be used a basis for the construction of preconditioners.

1 Introduction

It is well-known that any symmetric matrix \mathbf{X} , whether positive definite or not, can be factored

$$\mathbf{Q}^T \mathbf{X} \mathbf{Q} = \mathbf{L} \mathbf{D} \mathbf{L}^T$$

where \mathbf{D} is a micro-block diagonal matrix with blocks of dimension 1 or 2, \mathbf{L} is a unit lower triangular matrix, and \mathbf{Q} is a permutation matrix (see for instance [8, Section 4.4, page 115]).

There are various algorithms for the calculation of such a factorization, optimized for matrices \mathbf{X} which have a specific shape or satisfy specific properties. For instance, for an indefinite matrix \mathbf{X} without special structure, [3] presents the numerically stable construction of a permutation matrix \mathbf{Q} and the related matrices \mathbf{L} and \mathbf{D} . An even more economical pivoting strategy is presented in [2] and a Bunch-Kaufman-Parlett factorization implementation is presented in [14].

This paper focuses at indefinite linear systems of the form

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & -\mathbf{C} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix},$$

where the coefficient matrix is called \mathbf{X} and has a 2 by 2 block Karush-Kuhn-Tucker (KKT) structure with a potentially non-zero (2,2) block. For $\mathbf{C} = \mathbf{0}$, in equality-constraint quadratic optimization [20, page 40, Section 18.1], the coefficient matrix \mathbf{X} is called the KKT matrix. Matrices \mathbf{X} with block $\mathbf{C} = \mathbf{0}$ can also be found in mixed finite elements, Darcy's flow equations [1], problems of incompressible flow and elasticity [21], and many other application. The

case of $\mathbf{C} \neq \mathbf{0}$ and positive semi-definite arises in regularization and interior point methods in optimization, in electronic circuit simulation [23], and related applications.

The structure of \mathbf{X} has been exploited for the construction of preconditioners in many different ways [11, 12, 24, 9, 4, 15]. This paper closely follows the approach by [24] where it is assumed that \mathbf{X} has additional structure, i.e., that $\mathbf{B} = [\mathbf{B}_1, \mathbf{B}_2]$ is of maximal row rank and has upper triangular block \mathbf{B}_1 , which can be achieved through transformations of \mathbf{X} . However, whereas [24, Lemma 4.1] focuses on the construction of a Crout-type macro-block preconditioner $\hat{\mathbf{X}} = \hat{\mathbf{L}}\hat{\mathbf{D}}\hat{\mathbf{L}}^T$ (see also [7, Theorem 4.2]) based on the requirement that $\text{diag}(\mathbf{Q}^T\hat{\mathbf{X}}\mathbf{Q}) = \text{diag}(\mathbf{Q}^T\mathbf{X}\mathbf{Q})$ for a specific permutation matrix \mathbf{Q} (see [24, page 387]) we introduce a potentially non-zero \mathbf{C} block and actually calculate an explicit formula for the macro-block factorization $\mathbf{X} = \mathcal{L}\mathcal{D}\mathcal{L}^T$ based on the 2 by 2 and 1 by 1 micro-block Schilders' factorization in [18, 5, 6, 17, 24]. We show that for $\mathbf{C} = \mathbf{0}$ and upper triangular matrix $\text{diag}(\mathbf{B}_1) = \mathbf{I}$ our macro-block factorization is identical to the one in [24]. For non-zero \mathbf{C} we show that our macro-block factorization is unique and exists.

Many other important categories of preconditioning methods exist. For instance [11] assumes that one can factorize $\mathbf{C} = \mathbf{L}\mathbf{D}\mathbf{L}^T$, substitutes $\mathbf{x}_3 = -\mathbf{D}\mathbf{L}^T\mathbf{x}_2$, obtains the equivalent system

$$\begin{bmatrix} \mathbf{A} & \mathbf{0} & \mathbf{B}^T \\ \mathbf{0} & \mathbf{D}^{-1} & \mathbf{L}^T \\ \mathbf{B} & \mathbf{L} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix}$$

and considers preconditioners of the same block form, but with \mathbf{A} replaced by a symmetric preconditioner \mathbf{G} . (see also [18, 16, 22]). We mention this approach because also our approach requires the factorization of the positive semi-definite matrix \mathbf{C} , if it is non-diagonal.

The remainder of this paper introduces the factorization, its uniqueness, and existence as follows. Theorem 1 presents the micro-block factorization for indefinite problems, based on the micro-block structure presented in [24, Lemma 3.1]. Then, after presenting results on uniqueness, Theorem 2 provides an explicit formula for the factors of the induced macro-block factorization. Thereafter, Corollary 1 and Corollary 2 focus on the small difference and mostly similarities between macro-block factorization [24, Lemma 4.1] and our macro-block factorization (for $\mathbf{C} = \mathbf{0}$). We show that for $\mathbf{C} = \mathbf{0}$ and $\text{diag}(\mathbf{B}_1) = \mathbf{I}$ both macro-block factorizations are identical. Then Theorem 3 shows that the micro-block factorization (and hence related macro-block variant) exists for $\mathbf{C} > \mathbf{0}$, and that it is based on the existence of a symmetric positive definite Schur complement $\mathbf{A} + \mathbf{B}^T\mathbf{C}^{-1}\mathbf{B}$. Next, in Theorem 4 we prove the existence of our factorization for $\mathbf{C} = \mathbf{0}$, in a manner which differs from the proof in [24, Lemma 4.1]: We exploit the fact that our Crout-based macro-block factorization is unique under some conditions which makes it possible to assume even more structure of \mathbf{X} (in particular that $\mathbf{B}_1 = \mathbf{I}$ and $\mathbf{B}_2 = \mathbf{0}$), without loss of generality. We finish the existence proofs with Theorem 5, which shows the existence of our factorization for $\mathbf{C} = (0, \dots, 0, c_{d+1}, \dots, c_m)$ where c_{d+1}, \dots, c_m are positive. Finally Theorem 6 shows how to proceed for the general case where \mathbf{C} is symmetric positive definite but not diagonal.

2 The micro-block factorization

For use in the existence proofs later on, Definition 1 below formulates all shape-related conditions on \mathbf{X} and its blocks, as well as for the permutation p and permutation matrix \mathbf{Q} which induce the micro-block factorization. The existence proofs assume additional conditions, for instance that \mathbf{A} is positive definite (on the kernel of \mathbf{B}), that \mathbf{C} is positive semi-definite, and that \mathbf{B} is of maximal row rank.

Definition 1. Let n, m be natural positive numbers, let \mathbf{I}_n be the n by n identity matrix, and let $\mathbf{0}_{nm}$ be the n by m zero matrix. For the sake of convenience assume that $m \leq n$. Let \mathbf{A} be a symmetric n by n matrix, let

$$\mathbf{B} = [\mathbf{B}_1 \quad \mathbf{B}_2]$$

be an m by n matrix where \mathbf{B}_1 is an upper triangular m by m matrix and \mathbf{B}_2 an m by $n - m$ matrix. Let

$$\mathbf{C} = \text{diag}(c_{11}, \dots, c_{mm}), \quad c_{ii} \in \mathbb{R}, \quad 1 \leq i \leq m$$

be an m by m diagonal matrix. Let \mathbf{X} be partitioned into blocks which have shapes as follows:

$$\mathbf{X} = \begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & -\mathbf{C} \end{bmatrix} = \begin{bmatrix} \square & | & \square \\ \hline \square & | & \square \\ \hline \square & | & \square \end{bmatrix}$$

implicitly has a 3 by 3 macro-block structure. As in [24, page 386] we will use a permutation $p: \{1, \dots, n\} \mapsto \{1, \dots, n\}$ and without loss of generality assume that p is the identity map. With the use of this permutation we define the permutation matrix

$$\mathbf{Q} = [\mathbf{e}_{p(1)}, \mathbf{e}_{n+1}, \mathbf{e}_{p(2)}, \mathbf{e}_{n+2}, \dots, \mathbf{e}_{p(m)}, \mathbf{e}_{n+m}, \mathbf{e}_{p(m+1)}, \dots, \mathbf{e}_{p(n)}] \quad (1)$$

and define $\mathbf{Y} := \mathbf{Q}^T \mathbf{X} \mathbf{Q}$ to be the n by n micro-block matrix, just as in [24].

Note that by Definition 1 \mathbf{X} is symmetric which is necessary for the existence of a factorization of the form $\mathbf{X} = \mathbf{L} \circ \text{diag}^{-1}(\mathbf{L}) \circ \mathbf{L}^T$ which we construct in Theorem 1 where \mathbf{L} is a micro-block lower-triangular matrix and $\text{diag}(\mathbf{L})$ is its micro-block diagonal.

For the sake of illustration of how the micro-block factorization functions, consider an example which shows the micro-block partitioning of \mathbf{X} .

Example 1. Let $n = 7$, $m = 4$, and as in paper [24], assume that permutation $p: \{1, \dots, n\} \mapsto$

$\{1, \dots, n\}$ is the identity map. Then (row and column indices printed in the border of the matrix)

$$\mathbf{X} = \begin{array}{c} 1 \\ m \\ m+1 \\ n \\ n+1 \\ n+m \end{array} \begin{array}{c} 1 \\ m \\ m+1 \\ n \\ n+1 \\ n+m \end{array} \left(\begin{array}{cccc|cccc|cccc} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} & a_{17} & b_{11} & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} & a_{27} & b_{12} & b_{22} & 0 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} & a_{37} & b_{13} & b_{23} & b_{33} & 0 & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} & a_{47} & b_{14} & b_{24} & b_{34} & b_{44} & 0 \\ \hline a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & a_{56} & a_{57} & b_{51} & b_{52} & b_{53} & b_{54} & 0 \\ a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & a_{66} & a_{67} & b_{61} & b_{62} & b_{63} & b_{64} & 0 \\ a_{71} & a_{72} & a_{73} & a_{74} & a_{75} & a_{76} & a_{77} & b_{71} & b_{72} & b_{73} & b_{74} & 0 \\ \hline b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{16} & b_{17} & -c_{11} & 0 & 0 & 0 & 0 \\ 0 & b_{22} & b_{23} & b_{24} & b_{25} & b_{26} & b_{27} & 0 & -c_{22} & 0 & 0 & 0 \\ 0 & 0 & b_{33} & b_{34} & b_{35} & b_{36} & b_{37} & 0 & 0 & -c_{33} & 0 & 0 \\ 0 & 0 & 0 & b_{44} & b_{45} & b_{46} & b_{47} & 0 & 0 & 0 & 0 & -c_{44} \end{array} \right).$$

The permutation \mathbf{Q} is a product of two permutations: First, the rows $m+1, \dots, n$ of \mathbf{X} are swapped with some bottom rows (columns to the right-most columns):

$$\begin{array}{c} 1 \\ m \\ m+1 \\ 2m \\ 2m+1 \\ n+m \end{array} \begin{array}{c} 1 \\ m \\ m+1 \\ 2m \\ 2m+1 \\ n+m \end{array} \left(\begin{array}{cccc|cccc|cccc} a_{11} & a_{12} & a_{13} & a_{14} & b_{11} & 0 & 0 & 0 & a_{15} & a_{16} & a_{17} & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & b_{12} & b_{22} & 0 & 0 & a_{25} & a_{26} & a_{27} & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & b_{13} & b_{23} & b_{33} & 0 & a_{35} & a_{36} & a_{37} & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} & b_{14} & b_{24} & b_{34} & b_{44} & a_{45} & a_{46} & a_{47} & 0 \\ \hline b_{11} & b_{12} & b_{13} & b_{14} & -c_{11} & 0 & 0 & 0 & b_{15} & b_{16} & b_{17} & 0 \\ 0 & b_{22} & b_{23} & b_{24} & 0 & -c_{22} & 0 & 0 & b_{25} & b_{26} & b_{27} & 0 \\ 0 & 0 & b_{33} & b_{34} & 0 & 0 & -c_{33} & 0 & b_{35} & b_{36} & b_{37} & 0 \\ 0 & 0 & 0 & b_{44} & 0 & 0 & 0 & -c_{44} & b_{45} & b_{46} & b_{47} & 0 \\ \hline a_{51} & a_{52} & a_{53} & a_{54} & b_{15} & b_{25} & b_{35} & b_{45} & a_{55} & a_{56} & a_{57} & 0 \\ a_{61} & a_{62} & a_{63} & a_{64} & b_{16} & b_{26} & b_{36} & b_{46} & a_{65} & a_{66} & a_{67} & 0 \\ a_{71} & a_{72} & a_{73} & a_{74} & b_{17} & b_{27} & b_{37} & b_{47} & a_{75} & a_{76} & a_{77} & 0 \end{array} \right).$$

and next, its first $2m$ rows and columns are permuted with $(1 \ m+1 \ 2m+2 \ \dots \ m \ m+m \ 2m+1 \ \dots \ n)$ to obtain

$$\mathbf{Y} = \mathbf{Q}^T \mathbf{X} \mathbf{Q} = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 2m-1 \\ 2m \\ 2m+1 \\ n+m \end{array} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 2m-1 \\ 2m \\ 2m+1 \\ n+m \end{array} \left(\begin{array}{ccc|cccc|cccc} a_{11} & b_{11} & a_{12} & 0 & a_{13} & 0 & a_{14} & 0 & a_{15} & a_{16} & a_{17} & 0 \\ b_{11} & -c_{11} & b_{12} & 0 & b_{13} & 0 & b_{14} & 0 & b_{15} & b_{16} & b_{17} & 0 \\ a_{21} & b_{12} & a_{22} & b_{22} & a_{23} & 0 & a_{24} & 0 & a_{25} & a_{26} & a_{27} & 0 \\ 0 & 0 & b_{22} & -c_{22} & b_{23} & 0 & b_{24} & 0 & b_{25} & b_{26} & b_{27} & 0 \\ a_{31} & b_{13} & a_{32} & b_{23} & a_{33} & b_{33} & a_{34} & 0 & a_{35} & a_{36} & a_{37} & 0 \\ 0 & 0 & 0 & 0 & b_{33} & -c_{33} & b_{34} & 0 & b_{35} & b_{36} & b_{37} & 0 \\ a_{41} & b_{14} & a_{42} & b_{24} & a_{43} & b_{34} & a_{44} & b_{44} & a_{45} & a_{46} & a_{47} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & b_{44} & -c_{44} & b_{45} & b_{46} & b_{47} & 0 \\ \hline a_{51} & b_{15} & a_{52} & b_{25} & a_{53} & b_{35} & a_{54} & b_{45} & a_{55} & a_{56} & a_{57} & 0 \\ a_{61} & b_{16} & a_{62} & b_{26} & a_{63} & b_{36} & a_{64} & b_{46} & a_{65} & a_{66} & a_{67} & 0 \\ a_{71} & b_{17} & a_{72} & b_{27} & a_{73} & b_{37} & a_{74} & b_{47} & a_{75} & a_{76} & a_{77} & 0 \end{array} \right). \quad (2)$$

The resulting matrix (above) is (micro-block row and column indices printed in the border of the matrix)

$$\mathbf{Y} = \begin{array}{c} 1 \\ m \\ m+1 \\ n \end{array} \begin{array}{c} 1 \\ 2 \\ 3 \\ m \\ m+1 \\ n \end{array} \left(\begin{array}{cc|cc|cc|cc|cc|cc} a_{11} & b_{11} & a_{12} & 0 & a_{13} & 0 & a_{14} & 0 & a_{15} & a_{16} & a_{17} & 0 \\ b_{11} & -c_{11} & b_{12} & 0 & b_{13} & 0 & b_{41} & 0 & b_{15} & b_{16} & b_{17} & 0 \\ \hline a_{21} & b_{12} & a_{22} & b_{22} & a_{23} & 0 & a_{24} & 0 & a_{25} & a_{26} & a_{27} & 0 \\ 0 & 0 & b_{22} & -c_{22} & b_{23} & 0 & b_{24} & 0 & b_{25} & b_{26} & b_{27} & 0 \\ \hline a_{31} & b_{13} & a_{32} & b_{23} & a_{33} & b_{33} & a_{34} & 0 & a_{35} & a_{36} & a_{37} & 0 \\ 0 & 0 & 0 & 0 & b_{33} & -c_{33} & b_{34} & 0 & b_{35} & b_{36} & b_{37} & 0 \\ \hline a_{41} & b_{14} & a_{42} & b_{24} & a_{43} & b_{34} & a_{44} & b_{44} & a_{45} & a_{46} & a_{47} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & b_{44} & -c_{44} & b_{45} & b_{46} & b_{47} & 0 \\ \hline a_{51} & b_{15} & a_{52} & b_{25} & a_{53} & b_{35} & a_{54} & b_{45} & a_{55} & a_{56} & a_{57} & 0 \\ a_{61} & b_{16} & a_{62} & b_{26} & a_{63} & b_{36} & a_{64} & b_{46} & a_{65} & a_{66} & a_{67} & 0 \\ \hline a_{71} & b_{17} & a_{72} & b_{27} & a_{73} & b_{37} & a_{74} & b_{47} & a_{75} & a_{76} & a_{77} & 0 \end{array} \right). \quad (3)$$

By construction the micro-blocks of the matrix \mathbf{Y} have index ranges $i, j = 1, \dots, n$. As an example, matrix (2) has the micro-block entries in (3).

The micro-block partitioning shown in the example above stems from [24, pages 386, 387] and is at the core of the following micro-block factorization:

Theorem 1. *Let \mathbf{X} and its blocks \mathbf{A} , \mathbf{B} , and \mathbf{C} be as defined in Definition 1. Let matrix $\mathbf{Y} = \mathbf{Q}^\top \mathbf{X} \mathbf{Q}$ be micro-block indexed with indices $i, j = 1, \dots, n$ as defined in Definition 1. Then by construction of the permutation matrix \mathbf{Q} one finds that*

$$\mathbf{Y}_{ij} = \begin{bmatrix} a_{p(i),p(j)} & b_{j,p(i)} \\ b_{i,p(j)} & -c_{i,j} \end{bmatrix} \quad (4)$$

for all $1 \leq i \leq m$ and $1 \leq j \leq i$. Because \mathbf{B}_1 is upper triangular and \mathbf{C} is a diagonal matrix, more specifically

$$\mathbf{Y}_{ii} = \begin{bmatrix} a_{p(i),p(i)} & b_{i,p(i)} \\ b_{i,p(i)} & -c_{p(i),i} \end{bmatrix}, \quad \mathbf{Y}_{ij} = \begin{bmatrix} a_{p(i),p(j)} & b_{j,p(i)} \\ 0 & 0 \end{bmatrix}, \quad (5)$$

for all $1 \leq i \leq m$ and $1 \leq j < i$.

Let the n by n matrix $\mathbf{P}^\top \mathbf{E} \mathbf{P}$ be defined by its entries $e_{p(i),p(j)}$ as follows: First, define

$$e_{p(i),p(1)} = 0, \quad 1 \leq i \leq n, \quad (6)$$

and next, by column-recursion define for all $1 \leq j \leq i \leq m$

$$e_{p(i),p(j)} = \sum_{k=1}^{j-1} e_{p(i),p(k)}^{(k)} \quad (7)$$

with

$$e_{p(i),p(j)}^{(k)} = \begin{bmatrix} a_{p(i),p(k)} - e_{p(i),p(k)} \\ b_{k,p(i)} \end{bmatrix}^\top \begin{bmatrix} a_{p(k),p(k)} - e_{p(k),p(k)} & b_{k,p(k)} \\ b_{k,p(k)} & -c_{p(k),k} \end{bmatrix}^{-1} \begin{bmatrix} a_{p(j),p(k)} - e_{p(j),p(k)} \\ b_{k,p(j)} \end{bmatrix}, \quad (8)$$

(similarly for the other $1 \leq j \leq i \leq n$) under the assumption that the recursion does not break down. Observe that \mathbf{E} will be a lower triangular matrix. For $1 \leq i < j \leq m$ define $e_{p(i),p(j)} = 0$. Observe that the inverse of the matrix in (7) exists for $c_{kk} = 0$ if $b_{k,p(k)} \neq 0$.

Let

$$l_{p(i),p(j)} = a_{p(i),p(j)} - e_{p(i),p(j)}$$

and note that due to (7)

$$l_{p(i),p(j)} = a_{p(i),p(j)} - \sum_{k=1}^{j-1} \begin{bmatrix} l_{p(i),p(k)} \\ b_{k,p(i)} \end{bmatrix}^\top \begin{bmatrix} l_{p(k),p(k)} & b_{k,p(k)} \\ b_{k,p(k)} & -c_{kk} \end{bmatrix}^{-1} \begin{bmatrix} l_{p(j),p(k)} \\ b_{k,p(j)} \end{bmatrix}, \quad (9)$$

Then the column-recursion (7) does not break down if and only if there exists a micro-block lower triangular matrix \mathbf{L} of the form (3) such that

$$\mathbf{L} \circ \text{diag}^{-1}(\mathbf{L}) \circ \mathbf{L}^T = \mathbf{Y}. \quad (10)$$

The micro-blocks of \mathbf{L} are

$$\begin{aligned} \mathbf{L}_{ij} &= \mathbf{Y}_{ij} - \begin{bmatrix} e_{p(i),p(j)} & 0 \\ 0 & 0 \end{bmatrix}, & 1 \leq i \leq m, & 1 \leq j \leq i; \\ \mathbf{L}_{ij} &= \mathbf{Y}_{ij} - \begin{bmatrix} e_{p(i),p(j)} & 0 \end{bmatrix}, & m+1 \leq i \leq n, & 1 \leq j \leq m; \\ \mathbf{L}_{ij} &= \mathbf{Y}_{ij} - \begin{bmatrix} e_{p(i),p(j)} \end{bmatrix}, & m+1 \leq i, j \leq n. \end{aligned} \quad (11)$$

Furthermore, if the micro-block factorization exists, then it induces the macro-block factorization

$$\mathbf{X} = \mathbf{L}_X \mathbf{D}_X^{-1} \mathbf{L}_X^T \quad (12)$$

where

$$\mathbf{L}_X = \mathbf{Q} \mathbf{L} \mathbf{Q}^T = \begin{bmatrix} l_0(\mathbf{A} - \mathbf{E}) & \mathbf{B}^T \\ \text{diag}(\mathbf{B}) & -\mathbf{C} \end{bmatrix} =: \begin{bmatrix} \hat{\mathbf{L}} & \mathbf{B}^T \\ \text{diag}(\mathbf{B}) & -\mathbf{C} \end{bmatrix} \quad (13)$$

$$\mathbf{D}_X = \mathbf{Q} \text{diag}(\mathbf{L}) \mathbf{Q}^T = \begin{bmatrix} \text{diag}(\mathbf{A} - \mathbf{E}) & \text{diag}^T(\mathbf{B}) \\ \text{diag}(\mathbf{B}) & -\mathbf{C} \end{bmatrix} =: \begin{bmatrix} \hat{\mathbf{D}} & \text{diag}^T(\mathbf{B}) \\ \text{diag}(\mathbf{B}) & -\mathbf{C} \end{bmatrix} \quad (14)$$

where $l_0(\cdot)$ denotes the lower triangular part inclusive the diagonal, $\hat{\mathbf{D}} = \text{diag}(\hat{\mathbf{L}})$,

$$\text{diag}(\mathbf{B}) := [\text{diag}(\mathbf{B}_1) \quad \mathbf{0}_{m,n-m}]$$

and $\text{diag}^T(\mathbf{B}) := (\text{diag}(\mathbf{B}))^T$.

Proof. Below we use the notation of [24] except that we write \mathbf{L} instead of $\tilde{\mathbf{L}}$ and denote $\mathbf{Q}^T \mathbf{X} \mathbf{Q}$ by \mathbf{Y} . Furthermore, here \mathbf{L} stands for the micro-block lower triangular part, which includes the diagonal, which needs no special treatment.

Without loss of generality, assume that there \mathbf{Y} is a 4×4 micro-block matrix. First, assume that

$$\mathbf{L} \circ \text{diag}^{-T}(\mathbf{L}) \circ \mathbf{L}^T = \begin{bmatrix} \mathbf{L}_{11} & & & \\ \mathbf{L}_{21} & \mathbf{L}_{22} & & \\ \mathbf{L}_{31} & \mathbf{L}_{32} & \mathbf{L}_{33} & \\ \mathbf{L}_{41} & \mathbf{L}_{42} & \mathbf{L}_{43} & \mathbf{L}_{44} \end{bmatrix} \circ \begin{bmatrix} \mathbf{I}_2 & \mathbf{L}_{11}^{-T} \mathbf{L}_{21}^T & \mathbf{L}_{11}^{-T} \mathbf{L}_{31}^T & \mathbf{L}_{11}^{-T} \mathbf{L}_{41}^T \\ & \mathbf{I}_2 & \mathbf{L}_{22}^{-T} \mathbf{L}_{32}^T & \mathbf{L}_{22}^{-T} \mathbf{L}_{42}^T \\ & & \mathbf{I}_2 & \mathbf{L}_{33}^{-T} \mathbf{L}_{43}^T \\ & & & \mathbf{I}_2 \end{bmatrix} \quad (15)$$

where $\mathbf{L}_{ij}^T := (\mathbf{L}_{ij})^T$, $\mathbf{L}_{ij}^{-T} := (\mathbf{L}_{ij})^{-T}$, etc. Observe that the micro-blocks \mathbf{L}_{ij} can be calculated column for column: Let \mathbf{L}_k denote the k -th column of \mathbf{L} . Then

$$\mathbf{L}_1 \circ \mathbf{I}_2 = \mathbf{Y}_1 \implies \mathbf{L}_1 = \mathbf{Y}_1. \quad (16)$$

Next,

$$\mathbf{L}_1 \circ \mathbf{L}_{11}^{-\text{T}} \mathbf{L}_{21}^{\text{T}} + \mathbf{L}_2 \circ \mathbf{I}_2 = \mathbf{Y}_2 \implies \mathbf{L}_2 = \mathbf{Y}_2 - \mathbf{L}_1 \circ \mathbf{L}_{11}^{-\text{T}} \mathbf{L}_{21}^{\text{T}}.$$

This leads to the column-recursion (initialized with $\mathbf{L} = \mathbf{Y}$)

$$\mathbf{L}_j = \mathbf{Y}_j - \sum_{k=1}^{j-1} \mathbf{L}_k \mathbf{L}_{kk}^{-\text{T}} \mathbf{L}_{jk}^{\text{T}} \quad (17)$$

for all $1 \leq j \leq n$ which shows that column j of \mathbf{L} **only** depends on (entries of) the columns $k = 1, \dots, j-1$. The existence proofs later on exploit that \mathbf{L} can be determined column-wise.

The proof below is by induction with respect to the column index j , i.e., we will show that if (11) holds for columns $1 \leq j$ then it also holds for column $j+1$. For the sake of argument, without loss of generality, assume that $1 \leq j \leq i \leq m$. Then the induction hypothesis is: There exist scalars $e_{p(i),p(j)}$ such that

$$\mathbf{L}_{ij} = \mathbf{Y}_{ij} - \underbrace{\begin{bmatrix} e_{p(i),p(j)} & 0 \\ 0 & 0 \end{bmatrix}}_{\mathbf{E}_{p(i),p(j)}}, \quad 1 \leq j, \quad j \leq i \leq n. \quad (18)$$

Let \mathbf{v}_{ij} be the $e_{p(i),p(j)}$ -modified first column of $(\mathbf{L}_{ij})^{\text{T}}$, i.e.,

$$\mathbf{v}_{ij} := \begin{bmatrix} a_{p(i),p(j)} - e_{p(i),p(j)} \\ b_{j,p(i)} \end{bmatrix}, \quad 1 \leq j \leq m, \quad j \leq i \leq n \quad (19)$$

(for all $1 \leq j \leq m$ and $m+1 \leq i \leq n$ the first column is the only column and for all $m+1 \leq j \leq i \leq n$ it follows that $\mathbf{v}_{ij} = a_{p(i),p(j)} - e_{p(i),p(j)}$ is a scalar).

First note that the assumption holds for the first column of \mathbf{L} since $\mathbf{L}_1 = \mathbf{Y}_1$ due to (16). Now assume that the hypothesis holds for $1 \leq j$. The column-recursion (17) shows that

$$\mathbf{L}_{j+1} = \mathbf{Y}_{j+1} - \sum_{k=1}^j \mathbf{L}_k \mathbf{L}_{kk}^{-\text{T}} \mathbf{L}_{jk}^{\text{T}}$$

leads to $n-j$ independent ($j+1 \leq i \leq n$) entry-recursions ($\mathbf{L}_{i_1, j+1}$ does not depend on entry $\mathbf{L}_{i_2, j+1}$)

$$\mathbf{L}_{i,j+1} = \mathbf{Y}_{i,j+1} - \sum_{k=1}^j \mathbf{L}_{ik} \mathbf{L}_{kk}^{-\text{T}} \mathbf{L}_{jk}^{\text{T}}.$$

Since $k = 1, \dots, j$, by hypothesis it follows that

$$\begin{aligned} \mathbf{L}_{i,j+1} &\stackrel{(18)}{=} \mathbf{Y}_{i,j+1} - \sum_{k=1}^j (\mathbf{Y}_{ik} + \mathbf{E}_{ik}) (\mathbf{Y}_{kk} + \mathbf{E}_{kk})^{-\text{T}} (\mathbf{Y}_{jk} + \mathbf{E}_{jk})^{\text{T}} \\ &= \mathbf{Y}_{i,j+1} - \sum_{k=1}^j \begin{bmatrix} \mathbf{v}_{ik}^{\text{T}} \\ \mathbf{0} \end{bmatrix} (\mathbf{Y}_{kk} + \mathbf{E}_{kk})^{-\text{T}} [\mathbf{v}_{jk} \quad \mathbf{0}] \\ &= \mathbf{Y}_{i,j+1} - \sum_{k=1}^j \begin{bmatrix} \mathbf{v}_{ik}^{\text{T}} (\mathbf{Y}_{kk} + \mathbf{E}_{kk})^{-1} \mathbf{v}_{jk} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \end{aligned} \quad (20)$$

since $\mathbf{L}_{ik}\mathbf{L}_{kk}^{-\text{T}}\mathbf{L}_{jk}^{\text{T}}$ is the product of resp. a 2×1 , 1×1 and 1×2 block matrix, and because $\mathbf{Y}_{kk} + \mathbf{E}_{kk}$ is symmetric even if \mathbf{A} is not. This shows that the hypothesis holds for column $j + 1$ and that by construction

$$e_{p(i),p(j)} = \sum_{k=1}^{j-1} \mathbf{v}_{ik}^{\text{T}} (\mathbf{Y}_{kk} + \mathbf{E}_{kk})^{-1} \mathbf{v}_{jk}.$$

Observe that (7) in combination with $\mathbf{Y}_{ii} = \mathbf{Y}_{ii}^{\text{T}}$ implies that $\mathbf{L}_{ii} = \mathbf{L}_{ii}^{\text{T}}$, i.e.,

$$\text{diag}^{-\text{T}}(\mathbf{L}) = \text{diag}^{-1}(\mathbf{L}), \quad (21)$$

which leads to the desired result (10) which is both a Doolittle and Crout factorization.

Finally, (11) in combination with (5) show that only the \mathbf{A} -block related $[\mathbf{Y}_{ij}]_{11}$ entries of \mathbf{Y}_{ij} are updated. Based on this, relations (13) and (14) follow from the definition of \mathbf{L} , i.e., from the definition of the permutation (1). Let $\mathbf{l}_0(\mathbf{A})$ denote the lower triangular part of \mathbf{A} . Observe that $\mathbf{l}_0(\mathbf{A} - \mathbf{E}) = \mathbf{l}_0(\mathbf{A}) - \mathbf{E}$ because \mathbf{E} is lower triangular.

The head of the recursion (7) does not break down if the inverses of all

$$\begin{bmatrix} a_{p(k),p(k)} - e_{p(k),p(k)} & b_{k,p(k)} \\ b_{k,p(k)} & -c_{kk} \end{bmatrix}$$

exist. For $\mathbf{C} = \mathbf{0}$ this trivially holds since then the related determinants are non-zero if in addition $b_{k,p(k)} \neq 0$. \square

We need to show the existence of the factorization (10) and to show its uniqueness, which we start with.

Lemma 1. *Let \mathbf{A} be a symmetric square non-singular matrix. Then there exists at most one unique lower triangular (micro-)block matrix $\hat{\mathbf{L}}$ such that*

$$\mathbf{A} = \hat{\mathbf{L}} \circ \text{diag}^{-1}(\hat{\mathbf{L}}) \circ \hat{\mathbf{L}}^{\text{T}} \quad (22)$$

or equivalently there exists at most one unique lower triangular (micro-)block matrix \mathbf{L} with identity blocks on the diagonal and at most one non-singular diagonal (micro-)block matrix \mathbf{D} such that

$$\mathbf{A} = \mathbf{L} \circ \mathbf{D} \circ \mathbf{L}^{\text{T}}. \quad (23)$$

In addition, (micro-)block wise

$$\text{diag}(\mathbf{L}_1) = \mathbf{D}, \quad \mathbf{D} = \mathbf{D}^{\text{T}}. \quad (24)$$

This holds not only for the micro-block partition induced by (1) but for all block-partitions of \mathbf{A} . If \mathbf{A} is a square positive definite matrix then scalar-factorizations (22) and (23) exist.

Proof. Assume \mathbf{A} is a square matrix. The to be proven result is well-known for block-matrices where all blocks are 1 by 1 scalars. Below we demonstrate that the proof for the scalar case can be followed unaltered. For a block matrix \mathbf{L} let $\text{diag}(\mathbf{L})$ denote its (block-) diagonal. Then one can show

1. If \mathbf{L} is (block-) lower triangular with identity blocks (or scalars) on its diagonal then \mathbf{L} is non-singular, i.e., (block-) \mathbf{L}^{-1} exists, and \mathbf{L}^{-1} is lower triangular with identity blocks on its diagonal.
2. If \mathbf{L}_1 and \mathbf{L}_2 are block lower triangular then diagonal-block-wise

$$\text{diag}(\mathbf{L}_1\mathbf{L}_2) = \text{diag}(\mathbf{L}_1)\text{diag}(\mathbf{L}_2) \quad (25)$$

which implies that $\text{diag}(\mathbf{L}^{-1}) = \text{diag}(\mathbf{L})^{-1}$.

Now assume that there are two block factorizations of the form (23) (with lower triangular \mathbf{L}_1 , \mathbf{L}_2 with ones on the diagonal and non-singular diagonal \mathbf{D}_1 , \mathbf{D}_2):

$$\begin{aligned} \mathbf{L}_1\mathbf{D}_1\mathbf{L}_1^T &= \mathbf{L}_2\mathbf{D}_2\mathbf{L}_2^T \iff \\ \mathbf{L}_2^{-1}\mathbf{L}_1\mathbf{D}_1 &= \mathbf{D}_2\mathbf{L}_2^T\mathbf{L}_1^{-T} \implies \\ \text{diag}(\mathbf{L}_2^{-1}\mathbf{L}_1\mathbf{D}_1) &= \text{diag}(\mathbf{D}_2\mathbf{L}_2^T\mathbf{L}_1^{-T}) \iff_{(25)} \\ \text{diag}(\mathbf{D}_1) &= \text{diag}(\mathbf{D}_2). \end{aligned}$$

Let $\mathbf{D} = \mathbf{D}_1 = \mathbf{D}_2$. Now consider

$$\mathbf{L}_2^{-1}\mathbf{L}_1\mathbf{D} = \mathbf{D}\mathbf{L}_2^T\mathbf{L}_1^{-T}$$

where the left hand side matrix is a lower triangular and the right hand side matrix an upper triangular block matrix, i.e., they must be both identical to their diagonal, which is \mathbf{D} , i.e.,

$$\mathbf{L}_2^{-1}\mathbf{L}_1\mathbf{D} = \mathbf{D}, \mathbf{D}\mathbf{L}_2^T\mathbf{L}_1^{-T} = \mathbf{D} \implies \mathbf{L}_2^{-1}\mathbf{L}_1 = \mathbf{I}, \mathbf{L}_2^T\mathbf{L}_1^{-T} = \mathbf{I}$$

which also shows that $\mathbf{L}_1 = \mathbf{L}_2$. Finally, the equivalence of (22) and (23) follows from

$$\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{L}^T = (\mathbf{L}\mathbf{D})\mathbf{D}^{-1}(\mathbf{L}\mathbf{D})^T \stackrel{(25)}{=} (\mathbf{L}\mathbf{D})\text{diag}(\mathbf{L}\mathbf{D})^{-1}(\mathbf{L}\mathbf{D})^T.$$

That (24) holds for micro-block factorizations due to the special form of the update was shown in (21). However, it must hold for all symmetric matrices \mathbf{A} since

$$\mathbf{L}_1 \circ \text{diag}^{-1}(\mathbf{L}_1) \circ \mathbf{L}_1^T = \mathbf{A} = \mathbf{A}^T = \mathbf{L}_1 \circ \text{diag}^{-T}(\mathbf{L}_1) \circ \mathbf{L}_1^T.$$

Multiplication with \mathbf{L}_1^{-1} on the left, etc. leads to the desired result. The scalar factorization result for symmetric positive definite matrices \mathbf{A} is well-known. \square

Now we start to focus on the existence. We will show that the micro-block factorization exists for positive \mathbf{C} and for $\mathbf{C} = \mathbf{0}$.

3 The macro-block factorization

This section examines the similarities and differences with factorization [24, Lemma 4.1]. With a preconditioner derived from micro-block (10) factorization in mind, assuming that \mathbf{L}_1 and \mathbf{L}_2 are strictly lower triangular, [24, Lemma 4.1] proves that the macro-block factorization

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{B}_1^T & \mathbf{0} & \mathbf{L}_1 \\ \mathbf{B}_2^T & \mathbf{I}_{n-m} + \mathbf{L}_2 & \mathbf{M} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{D}_1 & \mathbf{0} & \mathbf{I} \\ \mathbf{0} & \mathbf{D}_2 & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{B}_1 & \mathbf{B}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{n-m} + \mathbf{L}_2^T & \mathbf{0} \\ \mathbf{L}_1^T & \mathbf{M}^T & \mathbf{I} \end{bmatrix} =: \mathcal{L}\mathcal{D}\mathcal{L}^T \quad (26)$$

exists (in paper [24], the rôles of \mathbf{B} and \mathbf{B}^T are reversed). Below Theorem 2 calculates the macro-block factorization (12) induced by micro-block factorization (10). Next, Corollary 1 shows that the induced macro-block factorization has macro blocks with identically shaped non-zero blocks (triangular, diagonal, rectangular) and mostly identical properties (for instance, both macro block 1, 3 are strictly lower diagonal). Finally, Corollary 2 proves that our induced macro-block factorization is identical to that presented in (26) if (necessary conditions) $\text{diag}(\mathbf{B}) = \mathbf{I}_m$ and $\mathbf{C} = \mathbf{0}$. In fact, if [24] had assumed that $\text{diag}(\mathbf{B}_1) = \mathbf{I}_m$ – which would not have restricted its presented factorization’s applicability – then the macro-block factorizations would have been identical. This paper induced macro-block factorization also holds if $\text{diag}(\mathbf{B}_1) \neq \mathbf{I}_m$.

Please note that for our micro-block induced macro-block factorization below in Theorem 2, similar to (26), we also label the blocks \mathbf{L}_1 , \mathbf{L}_2 and \mathbf{M} . However, except for special cases, these blocks differ from the like-wise named blocks in (26).

Theorem 2. *Let \mathbf{X} and its blocks \mathbf{A} , \mathbf{B} , and \mathbf{C} be as defined in Definition 1, i.e., \mathbf{A} is symmetric, \mathbf{B} is upper triangular, \mathbf{C} is diagonal. Let $\mathbf{L}_\mathbf{X}$, $\mathbf{D}_\mathbf{X}$ be defined as in (12). If the micro-block recursion 7 does not break down then there exists the macro-block factorization*

$$\mathbf{X} = \mathbf{L}_\mathbf{X}\mathbf{D}_\mathbf{X}^{-1}\mathbf{L}_\mathbf{X}^T = \begin{bmatrix} \mathbf{L}_1 & \mathbf{0} & \mathbf{B}_1^T \\ \mathbf{M} & \mathbf{L}_2 & \mathbf{B}_2^T \\ \text{d}\mathbf{B}_1 & \mathbf{0} & -\mathbf{C} \end{bmatrix} \begin{bmatrix} \mathbf{F}\mathbf{C} & \mathbf{0} & \mathbf{F}\text{d}\mathbf{B}_1 \\ \mathbf{0} & \mathbf{D}_2^{-1} & \mathbf{0} \\ \mathbf{F}\text{d}\mathbf{B}_1 & \mathbf{0} & -\mathbf{F}\mathbf{D}_1 \end{bmatrix} \begin{bmatrix} \mathbf{L}_1 & \mathbf{0} & \mathbf{B}_1^T \\ \mathbf{M} & \mathbf{L}_2 & \mathbf{B}_2^T \\ \text{d}\mathbf{B}_1 & \mathbf{0} & -\mathbf{C} \end{bmatrix}^T. \quad (27)$$

Define $\mathcal{L}_\mathbf{X} = \mathbf{L}_\mathbf{X}\mathbf{D}_\mathbf{X}^{-1}$ and $\mathcal{D}_\mathbf{X} = \mathbf{D}_\mathbf{X}$. Furthermore there exists the macro-block factorization

$$\mathbf{X} = \mathcal{L}_\mathbf{X}\mathcal{D}_\mathbf{X}\mathcal{L}_\mathbf{X}^T \quad \text{with } \mathcal{L}_\mathbf{X} \begin{bmatrix} \mathbf{B}_1^T\mathbf{F}\text{d}\mathbf{B}_1 + \mathbf{L}_1\mathbf{F}\mathbf{C} & \mathbf{0} & -\mathbf{B}_1^T\mathbf{F}\mathbf{D}_1 + \mathbf{L}_1\mathbf{F}\text{d}\mathbf{B}_1 \\ \mathbf{B}_2^T\mathbf{F}\text{d}\mathbf{B}_1 + \mathbf{M}\mathbf{F}\mathbf{C} & \mathbf{L}_2\mathbf{D}_2^{-1} & -\mathbf{B}_2^T\mathbf{F}\mathbf{D}_1 + \mathbf{M}\mathbf{F}\text{d}\mathbf{B}_1 \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix}. \quad (28)$$

Due to Lemma 1 the related micro-block factorizations are unique.

Proof. Let $\mathbf{L}_\mathbf{X}$, $\mathbf{D}_\mathbf{X}$ be defined as in (12), (13), and (14). By construction, if the recursion does not break down (i.e., if the micro-block factorization exists) then there exist diagonal m by m matrix \mathbf{D}_1 and diagonal $n - m$ by $n - m$ matrix \mathbf{D}_2 as well as a $n - m$ by m matrix \mathbf{M} , m by m lower triangular matrix \mathbf{L}_1 and $n - m$ by $n - m$ lower triangular matrix \mathbf{L}_2 such that, see (13)

and in addition (F3):

1. $[\mathcal{L}_X]_{12}, [\mathcal{L}_X]_{31}, [\mathcal{L}_X]_{32}$ are zero, i.e., $[\mathcal{L}_X]_{31}$ has zeros on its diagonal;
2. $[\mathcal{L}_X]_{33}$ is the identity matrix.

Reversely, if a macro-block \mathcal{L}_X matrix of the form (32) satisfies (F1) – (F3) then $\mathbf{Q}^T \mathcal{L}_X \mathbf{Q}$ is a micro-block lower triangular matrix with identity diagonal micro-blocks.

Proof. Consider \mathcal{L}_X of the factorization in (28):

$$\mathcal{L}_X \stackrel{(28)}{=} \begin{bmatrix} \mathbf{B}_1^T \mathbf{F} \mathbf{d} \mathbf{B}_1 + \mathbf{L}_1 \mathbf{F} \mathbf{C} & \mathbf{0} & -\mathbf{B}_1^T \mathbf{F} \mathbf{D}_1 + \mathbf{L}_1 \mathbf{F} \mathbf{d} \mathbf{B}_1 \\ \mathbf{B}_2^T \mathbf{F} \mathbf{d} \mathbf{B}_1 + \mathbf{M} \mathbf{F} \mathbf{C} & \mathbf{L}_2 \mathbf{D}_2^{-1} & -\mathbf{B}_2^T \mathbf{F} \mathbf{D}_1 + \mathbf{M} \mathbf{F} \mathbf{d} \mathbf{B}_1 \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_m \end{bmatrix}.$$

Note that \mathbf{D}_1 is the diagonal of \mathbf{L}_1 and \mathbf{D}_2 the diagonal of \mathbf{L}_2 . For an n by n square matrix \mathbf{A} let $\text{diag}(\mathbf{A})$ denote its diagonal matrix. Block $[\mathcal{L}_X]_{13}$ is lower triangular because \mathbf{B}_1^T and \mathbf{L}_1 are (and \mathbf{F} , \mathbf{D}_1 and $\mathbf{d} \mathbf{B}_1$ are diagonal) and it has a zero diagonal because its diagonal (matrix) is

$$\text{diag}([\mathcal{L}_X]_{13}) \stackrel{(25)}{=} -\text{diag}(\mathbf{B}_1) \mathbf{F} \mathbf{D}_1 + \text{diag}(\mathbf{L}_1) \mathbf{F} \mathbf{d} \mathbf{B}_1 = -\mathbf{d} \mathbf{B}_1 \mathbf{F} \mathbf{D}_1 + \mathbf{D}_1 \mathbf{F} \mathbf{d} \mathbf{B}_1 = \mathbf{0}_m.$$

Furthermore, since $\mathbf{D}_2 = \text{diag}(\mathbf{L}_2)$ one finds that

$$\text{diag}([\mathcal{L}_X]_{22}) = \text{diag}(\mathbf{L}_2) \mathbf{D}_2^{-1} = \mathbf{D}_2 \mathbf{D}_2^{-1} = \mathbf{I}_m$$

is a lower triangular matrix with ones on the diagonal and similarly

$$\text{diag}([\mathcal{L}_X]_{11}) = \mathbf{d} \mathbf{B}_1 \mathbf{F} \mathbf{d} \mathbf{B}_1 + \mathbf{D}_1 \mathbf{F} \mathbf{C} = (\mathbf{d} \mathbf{B}_1^2 + \mathbf{C} \mathbf{D}_1) \mathbf{F} = \mathbf{I}_m$$

is a lower triangular matrix with ones on the diagonal. \square

Corollary 2. Let \mathcal{L} be as defined in factorization (26), assume that $\text{diag}(\mathcal{L}_{13}) = \text{diag}(\mathbf{L}_1) = \mathbf{0}$. Let \mathcal{L}_X be as defined in factorization (28). If $\mathbf{C} = \mathbf{0}$ and $\text{diag}(\mathcal{L}_{11}) = \text{diag}(\mathbf{B}_1) = \mathbf{I}_m$ then $\mathcal{L} = \mathcal{L}_X$.

Proof. Assume that \mathcal{L} is a matrix of macro-block form (32)

$$\mathcal{L} = \begin{bmatrix} \begin{array}{|c|c|c|} \hline \triangle & & \triangle \\ \hline \text{---} & \triangle & \text{---} \\ \hline \end{array} \\ \hline \\ \hline \end{bmatrix}$$

which satisfies $\text{diag}(\mathcal{L}_{13}) = \text{diag}(\mathbf{L}_1) = \mathbf{0}$, $\text{diag}(\mathcal{L}_{31}) = \mathbf{0}$ and $\text{diag}(\mathcal{L}_{11}) = \text{diag}(\mathbf{B}_1) = \mathbf{I}$, $\text{diag}(\mathcal{L}_{33}) = \mathbf{I}$. Then its permuted form $\mathbf{Q}^T \hat{\mathbf{L}} \mathbf{Q}$ (1) is a lower-triangular micro-block matrix, (2) with identity matrices as its diagonal micro-blocks. Thus, by Lemma 1, $\mathcal{L}_X = \mathcal{L}$. \square

Note that properties (F2) and (F3) are explicitly resp. implicitly assumed for the proof of [24, Lemma 4.1]. Property (F1) is not necessarily met.

4 Existence and uniqueness of the factorizations

Now we show that the micro-block factorization exists for, in order, $\mathbf{C} > \mathbf{0}$, $\mathbf{C} = \mathbf{0}$ and $\mathbf{C} = (0, \dots, 0, c_{d+1}, \dots, c_n)$ where c_{d+1}, \dots, c_n are positive. First the case $\mathbf{C} > \mathbf{0}$.

Theorem 3. *Let \mathbf{X} and its blocks \mathbf{A} , \mathbf{B} , and \mathbf{C} be as defined in Definition 1. In addition, assume that \mathbf{A} is positive definite, $\mathbf{C} > \mathbf{0}$ and that \mathbf{B} is of maximal row rank. Then recursion (7) applied to \mathbf{X} does not break down and factorization (10) exists if the factorization*

$$\mathbf{A} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B} = \bar{\mathbf{L}} \circ \text{diag}^{-1}(\bar{\mathbf{L}}) \circ \bar{\mathbf{L}}^T$$

exist.

Thus, if \mathbf{A} is symmetric positive definite and \mathbf{C} is diagonal positive definite then the factorization (10) exists.

Proof. Assume that \mathbf{C} is positive diagonal. The Schur-complement \mathbf{S} of \mathbf{X}

$$\mathbf{S} = \mathbf{A} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B}$$

is positive definite (also for non-constant diagonal positive definite \mathbf{C} and for \mathbf{B} not of maximal row rank). Observe that for diagonal \mathbf{C} and upper triangular \mathbf{B} , since $j \leq i$,

$$s_{ij} := [\mathbf{A} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B}]_{ij} = a_{ij} + \sum_{k=1}^n b_{ki} c_{kk}^{-1} b_{kj} = a_{ij} + \sum_{k=1}^{\min(i,j,m)} b_{ki} c_{kk}^{-1} b_{kj} = \sum_{k=1}^{\min(j,m)} b_{ki} c_{kk}^{-1} b_{kj}. \quad (33)$$

Since the Schur complement is positive definite, due to Lemma 1 there exists a lower triangular matrix $\bar{\mathbf{L}}$ such that

$$\mathbf{S} = \bar{\mathbf{L}} \circ \text{diag}^{-1}(\bar{\mathbf{L}}) \circ \bar{\mathbf{L}}^T.$$

The recursion for the Schur complement and the micro-block factorization (10)

$$\mathbf{Y} = \mathbf{L} \circ \text{diag}^{-1}(\mathbf{L}) \circ \mathbf{L}^T$$

is similar: Due to (33), (4), and (17) for all $1 \leq j \leq i \leq m$ (note that now $\min(j, m) = j$)

$$\begin{aligned} s_{ij} &= a_{ij} + \sum_{k=1}^j b_{ki} c_{kk}^{-1} b_{kj} & \mathbf{Y}_{ij} &= \begin{bmatrix} a_{p(i),p(j)} & b_{j,p(i)} \\ b_{i,p(j)} & -c_{ij} \end{bmatrix} \\ \bar{l}_{ij} &= s_{ij} - \sum_{k=1}^{j-1} \bar{l}_{ik} (\bar{l}_{kk})^{-1} \bar{l}_{jk} & \mathbf{L}_{ij} &= \mathbf{Y}_{ij} - \sum_{k=1}^{j-1} \mathbf{L}_{ik} \mathbf{L}_{kk}^{-T} \mathbf{L}_{jk}^T. \end{aligned} \quad (34)$$

Observe that the sum in the Schur complement entry s_{ij} has one more entry $k = j$ than the sum in the recursion for \bar{l}_{ij} and \mathbf{L}_{ij} . Let the n by n matrix $(l_{ij})_{i,j=1}^n$ be defined as in (9).

Without loss of generality, assume that p is the identity map. The induction hypothesis is: Column-wise for columns $1 \leq j \leq n$:

$$\begin{aligned}\bar{\mathbf{l}}_j &= \mathbf{l}_j + \mathbf{b}_j \cdot b_{jj} \cdot c_{jj}^{-1}, & 1 \leq j \leq m, \\ \bar{\mathbf{l}}_j &= \mathbf{l}_j, & m+1 \leq j \leq n\end{aligned}\quad (35)$$

for all $j \leq i \leq n$.

The hypothesis holds for column 1: The first column of \mathbf{I}_1 and of $\bar{\mathbf{I}}_1$ are identical:

$$\bar{l}_{i1} = s_{i1} = a_{i1} + b_{1i} \cdot c_{11}^{-1} \cdot b_{11} = a_{i1} - 0 + b_{1i} \cdot b_{11} \cdot c_{11}^{-1} = l_{i1}$$

for all $1 \leq i \leq n$ (since $e_{i1} = 0$). Next, we assume that the hypothesis holds for a certain column and then show it holds for the next.

Define

$$\Delta_{ij} := b_{ji} \cdot \frac{b_{jj}}{c_{jj}},$$

then relation (35) implies

$$l_{ij} = \bar{l}_{ij} - \Delta_{ij}.$$

The micro-block diagonal blocks in (34) are

$$\begin{aligned}\mathbf{L}_{kk} &= \begin{bmatrix} l_{kk} & b_{kk} \\ b_{kk} & -c_{kk} \end{bmatrix} \implies \\ \mathbf{L}_{kk}^{-1} &= \frac{1}{-l_{kk}c_{kk} - b_{kk}^2} \begin{bmatrix} -c_{kk} & -b_{kk} \\ -b_{kk} & l_{kk} \end{bmatrix} = \frac{1}{c_{kk}\bar{l}_{kk}} \begin{bmatrix} c_{kk} & b_{kk} \\ b_{kk} & -(\bar{l}_{kk} - \Delta_{kk}) \end{bmatrix}.\end{aligned}$$

Now in relation (35) focus at the term (8), which is

$$e_{ij}^{(k)} := [\mathbf{L}_{ik} \mathbf{L}_{kk}^{-\text{T}} \mathbf{L}_{jk}^{\text{T}}]_{11}.$$

By direct calculation one finds:

$$\begin{aligned}e_{ij}^{(k)} &= \frac{1}{c_{kk}\bar{l}_{kk}} [\bar{l}_{ik} - \Delta_{ik} \quad b_{ki}] \begin{bmatrix} c_{kk} & b_{kk} \\ b_{kk} & -(\bar{l}_{kk} - \Delta_{kk}) \end{bmatrix} \begin{bmatrix} \bar{l}_{jk} - \Delta_{jk} \\ b_{kj} \end{bmatrix} \\ &= \frac{1}{c_{kk}\bar{l}_{kk}} [\bar{l}_{ik} - \Delta_{ik} \quad b_{ki}] \begin{bmatrix} c_{kk}(\bar{l}_{jk} - \Delta_{jk}) + b_{kk}b_{kj} \\ b_{kk}(\bar{l}_{jk} - \Delta_{jk}) - (\bar{l}_{kk} - \Delta_{kk})b_{kj} \end{bmatrix} \\ &= \frac{1}{c_{kk}\bar{l}_{kk}} (\bar{l}_{ik}c_{kk}\bar{l}_{jk} - \Delta_{jk}\bar{l}_{ik}c_{kk} - \Delta_{ik}\bar{l}_{jk}c_{kk} + \Delta_{ik}c_{kk}\Delta_{jk} + \bar{l}_{ik}b_{kk}b_{kj} \\ &\quad - \Delta_{ik}b_{kk}b_{kj} + \bar{l}_{jk}b_{kk}b_{ki} - \Delta_{jk}b_{ki}b_{kk} - \bar{l}_{kk}b_{ki}b_{kj} + \Delta_{kk}b_{ki}b_{kj})\end{aligned}$$

Of the last expression terms 2, 3, 4, and 8 cancel resp. term 5, 7, 6, and 10. This leaves

$$e_{ij}^{(k)} = \frac{1}{c_{kk}\bar{l}_{kk}} (\bar{l}_{ik}c_{kk}\bar{l}_{jk} - \bar{l}_{kk}b_{ki}b_{kj}) = \bar{l}_{ik}\bar{l}_{kk}^{-1}\bar{l}_{jk} - b_{ki}c_{kk}^{-1}b_{kj}. \quad (36)$$

Hence, one finds

$$\begin{aligned}
l_{ij} &= a_{ij} - \sum_{k=1}^{j-1} e_{ij}^{(k)} \\
&= a_{ij} - \sum_{k=1}^{j-1} \left(\bar{l}_{ik} \bar{l}_{kk}^{-1} \bar{l}_{jk} - b_{ki} c_{kk}^{-1} b_{kj} \right) \\
&= a_{ij} + \sum_{k=1}^{j-1} b_{ki} c_{kk}^{-1} b_{kj} - \sum_{k=1}^{j-1} \bar{l}_{ik} \bar{l}_{kk}^{-1} \bar{l}_{jk} \\
&= a_{ij} + \sum_{k=1}^j b_{ki} c_{kk}^{-1} b_{kj} - \sum_{k=1}^{j-1} \bar{l}_{ik} \bar{l}_{kk}^{-1} \bar{l}_{jk} - b_{ji} c_{jj}^{-1} b_{jj} \\
&= \bar{l}_{ij} - b_{ji} c_{jj}^{-1} b_{jj}
\end{aligned}$$

whence

$$l_{ij} + b_{ji} c_{jj}^{-1} b_{jj} = \bar{l}_{ij}$$

as was to be shown. The cases where $m \leq j \leq n$ can be similarly analyzed: For instance, consider l_{ij} for column $j = m + 1$ and rows i such that $j \leq i \leq n$. For $i > m$ all micro-blocks \mathbf{L}_{ij} are rectangular instead of square

$$\begin{bmatrix} a_{ij} & b_{ji} \end{bmatrix}$$

but the result follows in an similar manner because the related update terms $e_{ij}^{(k)}$ in (8) are identical, i.e., base on (36) for i with $j \leq i \leq n$

$$\begin{aligned}
\mathbf{L}_{ij} &= a_{ij} - \sum_{k=1}^{\min(j-1, m)} e_{ij}^{(k)} \\
&= a_{ij} - \sum_{k=1}^{\min(j-1, m)} \left(l_{ik} l_{kk}^{-1} l_{jk} - b_{ki} c_{kk}^{-1} b_{kj} \right) \\
&= a_{ij} + \sum_{k=1}^{\min(j-1, m)} b_{ki} c_{kk}^{-1} b_{kj} - \sum_{k=1}^{j-1} l_{ik} l_{kk}^{-1} l_{jk} \\
&= a_{ij} + \sum_{k=1}^m b_{ki} c_{kk}^{-1} b_{kj} - \sum_{k=1}^{j-1} l_{ik} l_{kk}^{-1} l_{jk} \\
&= l_{ij}.
\end{aligned}$$

For the columns $j > m + 1$ the updates are simple scalar products. By the result above, starting from column $j = m + 1$, one finds by induction

$$e_{ij}^{(k)} = \mathbf{L}_{ik} \mathbf{L}_{kk}^{-1} \mathbf{L}_{jk} = l_{ik} l_{kk}^{-1} l_{jk}$$

for all $k > m$. Thus, the result holds for all $1 \leq j \leq i \leq m$.

In block form (35) reads

$$\begin{aligned}\bar{\mathbf{L}} &= \begin{bmatrix} \mathbf{L}_1 & \mathbf{0}_{m,n-m} \\ \mathbf{M} & \mathbf{L}_2 \end{bmatrix} + [\mathbf{B}^T \quad \mathbf{0}_{n,n-m}] \begin{bmatrix} \text{diag}(\mathbf{B}_1)\mathbf{C}^{-1} & \mathbf{0}_{m,n-m} \\ \mathbf{0}_{n-m,m} & \mathbf{I}_{n-m} \end{bmatrix} \\ &= l_0(\mathbf{A}) - \mathbf{E} + [\mathbf{B}^T\mathbf{C}^{-1}\text{diag}(\mathbf{B}_1), \mathbf{0}_{n,n-m}]\end{aligned}$$

which implies that

$$\mathbf{E} = l_0(\mathbf{A}) + [\mathbf{B}^T\mathbf{C}^{-1}\text{diag}(\mathbf{B}_1), \mathbf{0}_{n,n-m}] - \bar{\mathbf{L}}$$

and therefore also that the micro-block factorization (10) exists: If the Schur-complement is uniquely factorized into $\mathbf{S} = \mathbf{L}_S\mathbf{D}_S\mathbf{L}_S^T$ where \mathbf{L}_S is lower triangular with ones on its diagonal, then

$$\begin{bmatrix} \mathbf{L}_1 & \mathbf{0}_{m,n-m} \\ \mathbf{M} & \mathbf{L}_2 \end{bmatrix} = \mathbf{L}_S - [\mathbf{B}^T\mathbf{C}^{-1}\text{diag}(\mathbf{B}_1), \mathbf{0}_{n,n-m}].$$

□

Lemma [24, Lemma 4.1] demonstrates the existence of a macro-block factorization (26), but not that it is unique. In fact, it is not unique: For $\text{diag}(\mathbf{B}_1) \neq \mathbf{I}$ micro-block factorization (10) induces a macro-block factorization (28) which differs from (26) – though all blocks have a non-zero structure similar to that of (26). To show that micro-block factorization (10) leads to a factorization of the form of [24, Lemma 4.1] (each of the 3×3 macro-blocks has the same zero, diagonal, lower triangular or rectangular shape), we proceed as follows.

Theorem 4. *Let \mathbf{X} and its blocks \mathbf{A} , \mathbf{B} , and \mathbf{C} be as defined in Definition 1. In addition, assume that \mathbf{A} is positive definite, $\mathbf{C} = \mathbf{0}$ and that \mathbf{B} is of maximal row rank. Then the micro-block factorization (10) exists for \mathbf{X} .*

Proof. First, for a transformed $\mathbf{V}^{-1}\mathbf{X}\mathbf{V}^{-T} =: \hat{\mathbf{X}} = \mathcal{L}_{\hat{\mathbf{X}}}\mathcal{D}_{\hat{\mathbf{X}}}\mathcal{L}_{\hat{\mathbf{X}}}^T$, we calculate the macro-block factorization related to our micro-block one. Then we show that the macro-block and hence the micro-block factorization exists. Thereafter, we back-transform and obtain existence and uniqueness for our micro-block factorization of \mathbf{X} itself, with macro block “lower triangular matrix” $\mathbf{V}\mathcal{L}_{\hat{\mathbf{X}}}$ and diagonal macro-block $\mathcal{D}_{\hat{\mathbf{X}}}$. Define \mathbf{V} as follows, note that it has ones on its main diagonal.

$$\mathbf{L}_B = \begin{bmatrix} \mathbf{B}_1^T d\mathbf{B}_1^{-1} & \mathbf{0} \\ \mathbf{B}_2^T d\mathbf{B}_1^{-1} & \mathbf{I}_{n-m} \end{bmatrix} \implies \mathbf{L}_B^{-1} = \begin{bmatrix} d\mathbf{B}_1\mathbf{B}_1^{-T} & \mathbf{0} \\ -\mathbf{B}_2^T\mathbf{B}_1^{-T} & \mathbf{I}_{n-m} \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} \mathbf{L}_B & \mathbf{0}_{n,m} \\ \mathbf{0}_{m,n} & \mathbf{I}_m \end{bmatrix}.$$

The matrix \mathbf{L}_B is implicitly used in the proof of [24, Lemma 4.1], except for the scaling factor $d\mathbf{B}_1^{-1}$. We add this factor to ensure that our macro-block factorization is uniquely related to a micro-block one. Define

$$\hat{\mathbf{X}} = \mathbf{V}^{-1}\mathbf{X}\mathbf{V}^{-T} = \begin{bmatrix} \hat{\mathbf{A}}_{11} & \hat{\mathbf{A}}_{12} & \hat{\mathbf{B}}_1^T \\ \hat{\mathbf{A}}_{21} & \hat{\mathbf{A}}_{22} & \hat{\mathbf{B}}_2^T \\ \hat{\mathbf{B}}_1 & \hat{\mathbf{B}}_2 & -\mathbf{C} \end{bmatrix} \quad (37)$$

where by construction

$$\begin{aligned}
\hat{\mathbf{A}} &= \begin{bmatrix} \hat{\mathbf{A}}_{11} & \hat{\mathbf{A}}_{12} \\ \hat{\mathbf{A}}_{21} & \hat{\mathbf{A}}_{22} \end{bmatrix} \\
&= \begin{bmatrix} d\mathbf{B}_1 \mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1} d\mathbf{B}_1 & d\mathbf{B}_1 \mathbf{B}_1^{-T} (-\mathbf{A}_{11} \mathbf{B}_1^{-1} \mathbf{B}_2 + \mathbf{A}_{12}) \\ (-\mathbf{B}_2^T \mathbf{B}_1^{-T} \mathbf{A}_{11} + \mathbf{A}_{21}) \mathbf{B}_1^{-1} d\mathbf{B}_1 & \mathbf{B}_2^T \mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1} \mathbf{B}_2 + \mathbf{A}_{22} - \mathbf{A}_{21} \mathbf{B}_1^{-1} \mathbf{B}_2 - \mathbf{B}_2^T \mathbf{B}_1^{-T} \mathbf{A}_{12} \end{bmatrix} \\
\hat{\mathbf{B}}_1 &= d\mathbf{B}_1 \\
\hat{\mathbf{B}}_2 &= \mathbf{0}_{m, n-m}.
\end{aligned} \tag{38}$$

Note that (37) holds based on

$$\begin{bmatrix} d\mathbf{B}_1 \mathbf{B}_1^{-T} & \mathbf{0} \\ -\mathbf{B}_2^T \mathbf{B}_1^{-T} & \mathbf{I}_{n-m} \end{bmatrix} \begin{bmatrix} \mathbf{B}_1^T \\ \mathbf{B}_2^T \end{bmatrix} = \begin{bmatrix} d\mathbf{B}_1 \\ \mathbf{0}_{m, n-m} \end{bmatrix}.$$

Note that $\mathbf{C} = \mathbf{0}_m$ and $\hat{\mathbf{B}}_1 = d\mathbf{B}_1$ imply that $\mathbf{F} = d\mathbf{B}_1^{-2}$. Thus the potential micro-block factorization (if the recursion does not break down) (27) produces macro-block factorization

$$\begin{aligned}
\hat{\mathbf{X}} = \mathbf{L}_{\hat{\mathbf{X}}} \mathbf{D}_{\hat{\mathbf{X}}}^{-1} \mathbf{L}_{\hat{\mathbf{X}}}^T &= \underbrace{\begin{bmatrix} \mathbf{L}_1 & \mathbf{0} & d\mathbf{B}_1 \\ \mathbf{M} & \mathbf{L}_2 & \mathbf{0} \\ d\mathbf{B}_1 & \mathbf{0} & \mathbf{0} \end{bmatrix}}_{\mathbf{L}_{\hat{\mathbf{X}}}} \circ \underbrace{\begin{bmatrix} \mathbf{0} & \mathbf{0} & d\mathbf{B}_1^{-1} \\ \mathbf{0} & \mathbf{D}_2^{-1} & \mathbf{0} \\ d\mathbf{B}_1^{-1} & \mathbf{0} & -d\mathbf{B}_1^{-1} \mathbf{D}_1 d\mathbf{B}_1^{-1} \end{bmatrix}}_{\mathbf{D}_{\hat{\mathbf{X}}}^{-1}} \circ \mathbf{L}_{\hat{\mathbf{X}}}^T \\
&= \underbrace{\begin{bmatrix} \mathbf{I}_m & \mathbf{0} & (\mathbf{L}_1 - \mathbf{D}_1) d\mathbf{B}_1^{-1} \\ \mathbf{0} & \mathbf{L}_2 \mathbf{D}_2^{-1} & \mathbf{M} d\mathbf{B}_1^{-1} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_m \end{bmatrix}}_{\mathcal{L}_{\hat{\mathbf{X}}}} \circ \mathbf{L}_{\hat{\mathbf{X}}}^T \\
&= \begin{bmatrix} \mathbf{L}_1 + \mathbf{L}_1^T - \mathbf{D}_1 & \mathbf{M}^T & d\mathbf{B}_1 \\ \mathbf{M} & \mathbf{L}_2 \mathbf{D}_2^{-1} \mathbf{L}_2^T & \mathbf{0} \\ d\mathbf{B}_1 & \mathbf{0} & \mathbf{0} \end{bmatrix}.
\end{aligned} \tag{39}$$

By construction (see (38)) $\hat{\mathbf{A}}_{11}$ and $\hat{\mathbf{A}}_{22}$ are symmetric positive definite whence $\text{lower}(\mathbf{L}_1) + \mathbf{D}_1 + \text{lower}(\mathbf{L}_1)^T$ uniquely partitions $\hat{\mathbf{A}}_{11}$ and $\mathbf{L}_2 \mathbf{D}_2 \mathbf{L}_2^T = \mathbf{L}_2 \text{diag}(\mathbf{L}_2)^{-1} \mathbf{L}_2^T$ is a unique factorization of, as in [24, Lemma 4.1]

$$\mathbf{L}_2 \mathbf{D}_2 \mathbf{L}_2^T = \hat{\mathbf{A}}_{22} = \begin{bmatrix} -\mathbf{B}_2^T \mathbf{B}_1^T & \mathbf{I}_{n-m} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} \begin{bmatrix} -\mathbf{B}_2^T \mathbf{B}_1^T & \mathbf{I}_{n-m} \end{bmatrix}^T$$

which latter matrix is symmetric positive definite. This shows that all of the blocks \mathbf{L}_1 , \mathbf{L}_2 , and \mathbf{M} exist, i.e., that the macro-block $\mathbf{L}_{\hat{\mathbf{X}}} \mathbf{D}_{\hat{\mathbf{X}}}^{-1} \mathbf{L}_{\hat{\mathbf{X}}}^T$ factorization for $\hat{\mathbf{X}}$ exists and its factors are uniquely determined.

Now consider the permuted, micro-block, form

$$\mathbf{Q}^T \hat{\mathbf{X}} \mathbf{Q} = (\mathbf{Q}^T \mathbf{L}_{\hat{\mathbf{X}}} \mathbf{Q}) (\mathbf{Q}^T \mathbf{D}_{\hat{\mathbf{X}}} \mathbf{Q})^{-1} (\mathbf{Q}^T \mathbf{L}_{\hat{\mathbf{X}}} \mathbf{Q})^T.$$

By construction $\mathbf{Q}^T \mathbf{D}_{\hat{\mathbf{X}}} \mathbf{Q}$ is a diagonal micro-block matrix, which is the diagonal of the lower triangular micro-block matrix $\mathbf{Q}^T \mathbf{L}_{\hat{\mathbf{X}}} \mathbf{Q}$. Thus, the factorization (10) exists for $\hat{\mathbf{X}}$, and equivalently, the recursion does not break down. (Note: The recursion breaks down if and only if the micro-block factorization does not exist).

Next, since \mathbf{V} is non-singular we know that the macro-block factorization

$$\mathbf{X} = \mathbf{V} \hat{\mathbf{X}} \mathbf{V}^T = (\mathbf{V} \mathcal{L}_{\hat{\mathbf{X}}}) \mathcal{D}_{\hat{\mathbf{X}}} (\mathbf{V} \mathcal{L}_{\hat{\mathbf{X}}})^T \quad (40)$$

exists where

$$\begin{aligned} \mathcal{L}_{\mathbf{X}} := \mathbf{V} \mathcal{L}_{\hat{\mathbf{X}}} &= \begin{bmatrix} \mathbf{B}_1^T d\mathbf{B}_1^{-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{B}_2^T d\mathbf{B}_1^{-1} & \mathbf{I}_{n-m} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_m \end{bmatrix} \circ \begin{bmatrix} \mathbf{I}_m & \mathbf{0} & (\mathbf{L}_1 - \mathbf{D}_1) d\mathbf{B}_1^{-1} \\ \mathbf{0} & \mathbf{L}_2 \mathbf{D}_2^{-1} & \mathbf{M} d\mathbf{B}_1^{-1} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_m \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{B}_1^T d\mathbf{B}_1^{-1} & \mathbf{0} & \mathbf{B}_1^T d\mathbf{B}_1^{-1} (\mathbf{L}_1 - \mathbf{D}_1) d\mathbf{B}_1^{-1} \\ \mathbf{B}_2^T d\mathbf{B}_1^{-1} & \mathbf{L}_2 \mathbf{D}_2^{-1} & \mathbf{B}_2^T d\mathbf{B}_1^{-1} (\mathbf{L}_1 - \mathbf{D}_1) d\mathbf{B}_1^{-1} + \mathbf{M} d\mathbf{B}_1^{-1} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_m \end{bmatrix}. \end{aligned} \quad (41)$$

To be shown is that this macro-block factorization represents *the* micro-block induced macro-block factorization 10 of \mathbf{X} . To this end it suffices that (after permutation) its micro-diagonal blocks are identity matrices. The entries which will form these micro-diagonal blocks stem from blocks $[\mathcal{L}_{\mathbf{X}}]_{11}$, $[\mathcal{L}_{\mathbf{X}}]_{22}$, $[\mathcal{L}_{\mathbf{X}}]_{33}$ (should have ones on their diagonal and be of lower triangular form) and blocks $[\mathcal{L}_{\mathbf{X}}]_{13}$, $[\mathcal{L}_{\mathbf{X}}]_{31}$ (should have zeros on their diagonal and be of lower triangular form). Inspection shows that this holds, for instance, since all factors are lower triangular

$$\text{diag}([\mathcal{L}_{\mathbf{X}}]_{13}) = \text{diag}(\mathbf{B}_1^T d\mathbf{B}_1^{-1}) \text{diag}(\mathbf{L}_1 - \mathbf{D}_1) \text{diag}(d\mathbf{B}_1^{-1}) = \mathbf{0},$$

and so forth. This shows that (40) is the macro-block equivalent of the micro-block factorization (10), which therefore exists. \square

As indicated, even for the case $\mathbf{C} = \mathbf{0}$ the matrix \mathbf{L}_1 in factorization 28 differs from \mathbf{L}_1 in factorization (26). Corollary (3) shows that for $\text{diag}(\mathbf{B}_1) = \mathbf{I}_m$ the difference is small.

Corollary 3. *Let $\text{diag}(\mathbf{B}_1) = \mathbf{I}_m$ and $\mathbf{C} = \mathbf{0}$. Observe that $\mathbf{L}_1 = l_0(\mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1})$ of our micro-block factorization (39) has diagonal $\mathbf{D}_1 > \mathbf{0}$, whereas $\mathbf{L}_1 = \mathbf{B}_1^T \text{lower}(\mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1})$ of [24] factorization 26 has diagonal $\mathbf{0}$. However, the 1, 3-blocks are identical:*

$$[\mathcal{L}_{\hat{\mathbf{X}}}]_{13} \stackrel{(41), \text{diag}(\mathbf{B}_1)=\mathbf{I}_m}{=} \mathbf{B}_1^T (\mathbf{L}_1 - \mathbf{D}_1) = \mathbf{B}_1^T \text{lower}(\mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1}) \stackrel{\mathbf{L}_1 \text{ in (26), Lemma 4.1}}{=} \mathcal{L}_{31}$$

according to [24, Lemma 4.1] (in [24] the rôles of \mathbf{B} and \mathbf{B}^T are reversed). Furthermore, our micro-block factorization directly applied to \mathbf{X} leads to $\mathcal{L}_{\mathbf{X}}$ defined in (28). That means that for that case

$$[\mathcal{L}_{\hat{\mathbf{X}}}]_{13} \stackrel{(41)}{=} -\mathbf{B}_1^T \mathbf{D}_1 + \mathbf{L}_1 \stackrel{\text{uniqueness}}{=} \mathbf{B}_1^T \text{lower}(\mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1}).$$

This is obviously the case for $\mathbf{L}_1 = \mathbf{B}_1^T l_0 (\mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1})$ and $\mathbf{D}_1 = \text{diag}(\mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1})$ for which

$$\text{diag}(\mathbf{L}_1) = \text{diag}(\mathbf{B}_1) \text{diag}(l_0 (\mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1})) = \text{diag}(\mathbf{B}_1^{-T} \mathbf{A}_{11} \mathbf{B}_1^{-1}) = \mathbf{D}_1.$$

There is a similar relationship between \mathbf{L}_2 in (28) and \mathbf{L}_2 in (26).

Theorem 5. Let \mathbf{X} and its blocks \mathbf{A} , \mathbf{B} , and \mathbf{C} be as defined in Definition 1. In addition, assume that \mathbf{A} is positive definite and that $\mathbf{C} = \text{diag}(0, 0, \dots, c_{d-1, d-1}, \dots, c_{mm})$ contains first d zeros and next $m - d$ positive real numbers. Assume that \mathbf{B} is of maximal row rank. Then the micro-block factorization (10) exists for \mathbf{X} .

Proof. Let \mathbf{L}_B , \mathbf{V} and $\hat{\mathbf{X}}$ be as defined in (4). We show that the micro-block factorization exists for $\hat{\mathbf{Y}} = \mathbf{Q}^T \hat{\mathbf{X}} \mathbf{Q}$ which implies that the macro-block factorization exists for $\hat{\mathbf{X}}$ and hence by Theorem 4, using the argumentation from (40) onwards, also for \mathbf{X} .

Without loss of generality, assume that p is the identity map. Let d be a positive natural number and assume that the first d diagonal entries of \mathbf{C} are zero. Focus on l_{ij} in (9), which depends on the update term $e_{ij}^{(k)}$ in (8). By direct calculation one finds (since $k < \min(i, j)$ implies $b_{ki} = b_{kj} = 0$):

$$\begin{aligned} e_{ij}^{(k)} &= [\mathbf{L}_{ik} \mathbf{L}_{kk}^{-T} \mathbf{L}_{jk}^T]_{11} \\ &= [l_{ik} \ 0] \begin{bmatrix} l_{kk} & b_{kk} \\ b_{kk} & -c_{kk} \end{bmatrix}^{-1} \begin{bmatrix} l_{jk} \\ 0 \end{bmatrix} \\ &= \frac{1}{c_{kk} l_{kk} + b_{kk}^2} [l_{ik} \ 0] \begin{bmatrix} c_{kk} & b_{kk} \\ b_{kk} & -l_{kk} \end{bmatrix} \begin{bmatrix} l_{jk} \\ 0 \end{bmatrix} \\ &= \frac{l_{ik} c_{kk} l_{jk}}{c_{kk} l_{kk} + b_{kk}^2} \implies \\ l_{ij} &= a_{ij} - \sum_{k=1}^{j-1} \frac{l_{ik} c_{kk} l_{jk}}{c_{kk} l_{kk} + b_{kk}^2}. \end{aligned} \tag{42}$$

Therefore, by construction $l_{ij} = a_{ij}$ exists (here we use that \mathbf{B} is upper triangular and of maximal row rank) for all $1 \leq j \leq d+1$, $1 \leq i \leq n$. This shows that, consistent with Theorem 4, that the first $d+1$ columns of matrix $(l_{ij})_{i,j=1}^n$ are the first $d+1$ columns of $\hat{\mathbf{A}}$.

Now we have to examine what happens if the micro-block column-recursion continues with column $d+2$ and onward – note that only the square part (MATLAB notation) $\hat{\mathbf{Y}}(d+1 : n, d+1 : n)$ is involved. For the sake of argument, without loss of generality, consider the case $d = 1$, $n = 7$, $m = 4$, and the matrix $\hat{\mathbf{Y}}$ in (2) with the first micro-block row and column deleted (after the determination of the first $d+1$ columns of $(l_{ij})_{i,j=1}^n$ in (42)):

$$\hat{\mathbf{Y}}_{-d} := \left[\begin{array}{cccccc|ccc} a_{22} & b_{22} & a_{23} & 0 & a_{24} & 0 & a_{25} & a_{26} & a_{27} \\ b_{22} & -c_{22} & b_{23} & 0 & b_{24} & 0 & b_{25} & b_{26} & b_{27} \\ a_{32} & b_{23} & a_{33} & b_{33} & a_{34} & 0 & a_{35} & a_{36} & a_{37} \\ 0 & 0 & b_{33} & -c_{33} & b_{34} & 0 & b_{35} & b_{36} & b_{37} \\ a_{42} & b_{24} & a_{43} & b_{34} & a_{44} & b_{44} & a_{45} & a_{46} & a_{47} \\ 0 & 0 & 0 & 0 & b_{44} & -c_{44} & b_{45} & b_{46} & b_{47} \\ \hline a_{52} & b_{25} & a_{53} & b_{35} & a_{54} & b_{45} & a_{55} & a_{56} & a_{57} \\ a_{62} & b_{26} & a_{63} & b_{36} & a_{64} & b_{46} & a_{65} & a_{66} & a_{67} \\ a_{72} & b_{27} & a_{73} & b_{37} & a_{74} & b_{47} & a_{75} & a_{76} & a_{77} \end{array} \right]. \tag{43}$$

This matrix turns out to be related to

$$\hat{\mathbf{X}}_{-d} = \mathbf{Q}_{-d} \hat{\mathbf{Y}}_{-d} \mathbf{Q}_{-d}^T = \left[\begin{array}{cccccc|ccc} a_{22} & a_{23} & a_{24} & a_{25} & a_{26} & a_{27} & b_{22} & 0 & 0 \\ a_{32} & a_{33} & a_{34} & a_{35} & a_{36} & a_{37} & b_{23} & b_{33} & 0 \\ a_{42} & a_{43} & a_{44} & a_{45} & a_{46} & a_{47} & b_{24} & b_{34} & b_{44} \\ a_{52} & a_{53} & a_{54} & a_{55} & a_{56} & a_{57} & b_{25} & b_{35} & b_{45} \\ a_{62} & a_{63} & a_{64} & a_{65} & a_{66} & a_{67} & b_{26} & b_{36} & b_{46} \\ a_{72} & a_{73} & a_{74} & a_{75} & a_{76} & a_{77} & b_{27} & b_{37} & b_{47} \\ \hline b_{22} & b_{23} & b_{24} & b_{25} & b_{26} & b_{27} & -c_{22} & 0 & 0 \\ 0 & b_{33} & b_{34} & b_{35} & b_{36} & b_{37} & 0 & -c_{33} & 0 \\ 0 & 0 & b_{44} & b_{45} & b_{46} & b_{47} & 0 & 0 & -c_{44} \end{array} \right] = \begin{bmatrix} \tilde{\mathbf{A}} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \tilde{\mathbf{C}} \end{bmatrix}$$

which is identical to matrix $\hat{\mathbf{X}}$ with columns and rows $1, n+1$ deleted. The blocks of \mathbf{X}_{-d} satisfy: $\tilde{\mathbf{A}}$ is positive definite, $\tilde{\mathbf{B}}$ has full row rank and is upper triangular, and $\tilde{\mathbf{C}} > \mathbf{0}$. Hence, by Theorem 3 the micro-block factorization of $\hat{\mathbf{Y}}_{-d}$ in (43) exists. Let the lower triangular coefficients related to \mathbf{Y}_{-d} defined in (9) be denoted with $l_{ij}^{(-d)}$. Then since $e_{ij} = 0$ for $1 \leq j \leq d$, $j \leq i \leq n$ it straightforwardly follows that $l_{i,j+d} = l_{ij}^{(-d)}$ for all $d+1 \leq j \leq n$ and $j \leq i \leq n$. Hence the micro-block factorization of $\hat{\mathbf{X}}$ exists.

Finally, as in Theorem 4 one can show that the micro block factorization for \mathbf{X} exists as well. \square

For the case that \mathbf{B} is not upper triangular (but is of maximal row rank) and that \mathbf{C} is not a (non-negative) diagonal matrix it is possible to ensure these properties at the additional costs of two to be calculated factorizations, as is indicated in [24]. The approach for non-upper triangular \mathbf{B} is taken from [24, above Lemma 4.1]. Theorem 6 extends it for non-diagonal (square) $\mathbf{C} \neq \mathbf{0}$.

Theorem 6. *Let \mathbf{X} and its blocks \mathbf{A} , \mathbf{B} , and \mathbf{C} be as defined in Definition 1. In addition, assume that \mathbf{A} is positive definite, \mathbf{C} is positive definite but not necessarily diagonal, and that \mathbf{B} is of maximal row rank, but not necessarily upper triangular. Then, there exists an orthogonal matrix \mathbf{V}_B , and a non-singular matrix \mathbf{V}_C with positive diagonal, a micro-block related permutation matrix \mathbf{Q} , and a micro-factorizable matrix $\hat{\mathbf{X}} := \mathbf{L}_{\hat{\mathbf{X}}} \circ \text{diag}^{-1}(\mathbf{L}_{\hat{\mathbf{X}}}) \circ \mathbf{L}_{\hat{\mathbf{X}}}^T$ such that*

$$\mathbf{X} = \begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & -\mathbf{C} \end{bmatrix} = \mathbf{V}_C \mathbf{V}_B^T \mathbf{Q} \mathbf{L}_{\hat{\mathbf{X}}} \circ \text{diag}^{-1}(\mathbf{L}_{\hat{\mathbf{X}}}) \circ \mathbf{L}_{\hat{\mathbf{X}}}^T \mathbf{Q}^T \mathbf{V}_B \mathbf{V}_C^{-1}.$$

Proof. First, since \mathbf{C} is symmetric positive definite there exists a unique factorization $\mathbf{C} = \mathcal{L}_C \mathcal{D}_C \mathcal{L}_C^T$ where \mathcal{L}_C is lower triangular with positive diagonal entries and $\mathcal{D}_C = \mathbf{I}$. Let $\hat{\mathbf{C}} = \mathcal{L}_C$. Next, from a QR decomposition of $\mathbf{B}^T \mathcal{L}_C^{-T}$ one can derive that there exists an n by n permutation matrix Π and an orthogonal m by m matrix \mathbf{Q} such that

$$\mathbf{B}^T \mathcal{L}_C^{-T} = \begin{bmatrix} \mathbf{B}_1^T \\ \mathbf{B}_2^T \end{bmatrix} \mathcal{L}_C^{-T} = \Pi \hat{\mathbf{B}}^T \mathbf{Q}$$

where $\hat{\mathbf{B}}$ is upper triangular and of maximal row rank, i.e., satisfies the conditions in Definition 1. Finally, let $\hat{\mathbf{A}} = \Pi \mathbf{A} \Pi^T$, observe that $\hat{\mathbf{C}} := \hat{\mathbf{Z}} \mathcal{D}_C \hat{\mathbf{Z}}^T = \mathcal{D}_C$, define

$$\mathbf{V}_C = \begin{bmatrix} \mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & \mathcal{L}_C \end{bmatrix}, \quad \mathbf{V}_B = \begin{bmatrix} \Pi & \mathbf{0} \\ \mathbf{0} & \mathbf{Q} \end{bmatrix}, \quad \hat{\mathbf{X}} = \begin{bmatrix} \hat{\mathbf{A}} & \hat{\mathbf{B}}^T \\ \hat{\mathbf{B}} & -\hat{\mathbf{C}} \end{bmatrix},$$

and note that the latter matrix can be micro-block factorized due to Theorem 3. Without loss of generality, assume that Π^T defines the permutation $p: \{1, \dots, n\} \mapsto \{1, \dots, n\}$ and define

$$\mathbf{Q} = [\mathbf{e}_1, \mathbf{e}_{n+1}, \mathbf{e}_2, \mathbf{e}_{n+2}, \dots, \mathbf{e}_m, \mathbf{e}_{n+m}, \mathbf{e}_{m+1}, \dots, \mathbf{e}_n]. \quad (44)$$

Then

$$\mathbf{Q}^T \mathbf{V}_B \mathbf{V}_C^{-1} \mathbf{X} \mathbf{V}_C^{-T} \mathbf{V}_B^T \mathbf{Q} = \mathbf{Q}^T \begin{bmatrix} \hat{\mathbf{A}} & \hat{\mathbf{B}}^T \\ \hat{\mathbf{B}} & -\hat{\mathbf{C}} \end{bmatrix} \mathbf{Q} = \mathbf{Q}^T \hat{\mathbf{X}} \mathbf{Q} = \mathbf{L}_{\hat{\mathbf{X}}} \circ \text{diag}^{-1}(\mathbf{L}_{\hat{\mathbf{X}}}) \circ \mathbf{L}_{\hat{\mathbf{X}}}^T$$

yields the desired result. \square

The case of non-diagonal symmetric positive semi-definite matrix \mathbf{C} can be treated similarly, based on the following result from [13], [10], and [19]: Let the n by n matrix \mathbf{A} be symmetric positive semi-definite and of rank $r \leq n$.

1. There exists at least one upper triangular \mathbf{R} with nonnegative diagonal elements such that $\mathbf{A} = \mathbf{R}^T \mathbf{R}$;
2. There exists a permutation matrix Π such that matrix $\Pi^T \mathbf{A} \Pi$ has a unique Choleski decomposition

$$\Pi^T \mathbf{A} \Pi = \mathbf{R}^T \mathbf{R}$$

where

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

has is upper triangular r by r block \mathbf{R}_{11} , which has positive diagonal elements.

Since we assume that the first d diagonal elements of \mathbf{C} are zero – and not the last ones – this result needs to be combined with an additional permutation.

5 Numerical examples

As an example consider a variant on [25, Example 5.3], and focus on the cases $\mathbf{C} > \mathbf{0}$, $\mathbf{C} \geq \mathbf{0}$, and $\mathbf{C} = \mathbf{0}$, for a matrix \mathbf{B} with $\text{diag}(\mathbf{B}_1) \neq \mathbf{I}_m$.

Example 2. The case $\mathbf{C} > \mathbf{0}$: Identical to the first case in [25, Example 5.3] we choose $\gamma_1 = 1$ and $\gamma_2 = 2$ for the matrix \mathbf{C} below. In addition we alter \mathbf{B} such that it is of full row rank:

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 3 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 5 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} \gamma_1 & 0 & 0 \\ 0 & \gamma_2 & 0 \\ 0 & 0 & 3 \end{bmatrix}.$$

Note that \mathbf{A} and \mathbf{C} are symmetric positive definite and that $\text{diag}(\mathbf{B}_1) \neq \mathbf{I}_m$. Based on these blocks one finds

$$\mathbf{X} \stackrel{\text{Definition 1}}{=} \left[\begin{array}{cccc|ccc} 2 & 1 & 0 & 0 & 2 & 0 & 0 \\ 1 & 3 & 1 & 0 & 0 & 3 & 0 \\ 0 & 1 & 4 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 5 & 0 & 0 & 1 \\ \hline 2 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & -3 \end{array} \right], \quad \mathbf{Y} \stackrel{(10)}{=} \left[\begin{array}{ccc|cc|cc} 2 & 2 & 1 & 0 & 0 & 0 & 0 \\ 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ \hline 1 & 0 & 3 & 3 & 1 & 0 & 0 \\ 0 & 0 & 3 & -2 & 0 & 0 & 0 \\ \hline 0 & 0 & 1 & 0 & 4 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & -3 & 1 \\ \hline 0 & 0 & 0 & 0 & 1 & 1 & 5 \end{array} \right]$$

and calculation shows, rounded to three decimal places, that in macro-block form

$$\mathbf{L}_\mathbf{X} \stackrel{(13),(27)}{=} \left[\begin{array}{ccc|c|ccc} 2 & 0 & 0 & 0 & 2 & 0 & 0 \\ 1 & 2.833 & 0 & 0 & 0 & 3 & 0 \\ 0 & 1 & 3.864 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 1 & 4.910 & 0 & 0 & 1 \\ 2 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -3 \end{array} \right], \quad \mathbf{D}_\mathbf{X} \stackrel{(14),(27)}{=} \left[\begin{array}{ccc|c|ccc} 2 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 2.833 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 3.864 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 4.910 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -3 \end{array} \right].$$

As claimed, $\mathbf{L}_\mathbf{X}$ contains blocks \mathbf{B}_1^T , \mathbf{B}_2^T and $\text{diag}(\mathbf{B}_1)$ respectively at blocks (1,3), (2,3) and (3,1) and so forth. Furthermore, the diagonals of $\mathbf{D}_\mathbf{X}$ and $\mathbf{L}_\mathbf{X}$ in blocks (1,1), (1,3), (3,1), (3,3), and (2,2) are identical as they should be according to Theorem 1. The related matrix $\mathcal{L}_\mathbf{X}$ turns out to be

$$\mathcal{L}_\mathbf{X} \stackrel{(28)}{=} \left[\begin{array}{ccc|c|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.167 & 1 & 0 & 0 & 0.333 & 0 & 0 \\ 0 & 0.136 & 1 & 0 & 0 & 0.205 & 0 \\ \hline 0 & 0 & 0.318 & 1 & 0 & 0 & -0.227 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right].$$

This matrix contains ones at its main diagonal, and zeros at the diagonals of its blocks (1,3) and (3,1), as it should have due to Corollary 1.

Example 3. The case $\mathbf{C} \geq \mathbf{0}$: The blocks \mathbf{A} and \mathbf{B} are as in Example 2. We take $\gamma_1 = 0$ and $\gamma_2 = 2$ as in the second case of [25, Example 5.3]. Therefore matrix \mathbf{X} and \mathbf{Y} are identical to those in Example 2, except for entry (5,5), respectively 2×2 micro-block entry (1,1). For this example one finds, rounded to three decimal places

$$\mathbf{L}_\mathbf{X} \stackrel{(13),(27)}{=} \left[\begin{array}{ccc|c|ccc} 2 & 0 & 0 & 0 & 2 & 0 & 0 \\ 1 & 3 & 0 & 0 & 0 & 3 & 0 \\ 0 & 1 & 3.867 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 4.910 & 0 & 0 & 1 \\ \hline 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -3 \end{array} \right], \quad \mathcal{L}_\mathbf{X} \stackrel{(28)}{=} \left[\begin{array}{ccc|c|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0.500 & 0 & 0 \\ 0 & 0.133 & 1 & 0 & 0 & 0.200 & 0 \\ \hline 0 & 0 & 0.317 & 1 & 0 & 0 & -0.228 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right].$$

Example 4. The case $\mathbf{C} = \mathbf{0}$: The blocks \mathbf{A} and \mathbf{B} are as in Example 2. We take $\gamma_1 = 0$ and $\gamma_2 = 0$ as in the third case of [25, Example 5.3]. For this last example one finds, rounded to three decimal places

$$\mathbf{L}_\mathbf{X} \stackrel{(13),(27)}{=} \left[\begin{array}{ccc|c|ccc} 2 & 0 & 0 & 0 & 2 & 0 & 0 \\ 1 & 3 & 0 & 0 & 0 & 3 & 0 \\ 0 & 1 & 4 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 1 & 7 & 0 & 0 & 1 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{array} \right], \quad \mathcal{L}_\mathbf{X} \stackrel{(28)}{=} \left[\begin{array}{ccc|c|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0.500 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0.333 & 0 \\ \hline 0 & 0 & 1 & 1 & 0 & 0 & -3 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right].$$

In this case one finds that \mathcal{L} and \mathcal{D} of (26) are – calculated explicitly from the formulas for the blocks \mathbf{L}_1 , \mathbf{L}_2 , \mathbf{M} , \mathbf{L}_2 and \mathbf{D}_2 in [24, Lemma 4.1]:

$$\mathcal{L} \underset{(26)}{=} \left[\begin{array}{ccc|ccc} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0.500 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0.333 \\ \hline 0 & 0 & 1 & 1 & 0 & -3 \\ \hline 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right], \quad \mathcal{D} \underset{(26)}{=} \left[\begin{array}{ccc|ccc} 0.500 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0.333 & 0 & 0 & 0 & 1 \\ 0 & 0 & 4 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 7 & 0 & 0 \\ \hline 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{array} \right].$$

The main the difference with Schilders' factorization factor \mathcal{L} of (26) (from [24, Lemma 4.1]) is that $\mathcal{L}_{11} = \mathbf{B}_1$ and $\mathcal{L}_{31} = \mathbf{0}_m$ whereas $[\mathcal{L}_{\mathbf{X}}]_{11} = \mathbf{B}_1$ but $[\mathcal{L}_{\mathbf{X}}]_{31} \neq \mathbf{0}_m$ and reversely $[\mathbf{L}_{\mathbf{X}}]_{11} \neq \mathbf{B}_1$ but $[\mathbf{L}_{\mathbf{X}}]_{31} = \mathbf{0}_m$. For matrices \mathbf{B} with $\text{diag}(\mathbf{B}_1) = \mathbf{I}_m$ one would obtain $\mathcal{L} = \mathcal{L}_{\mathbf{X}}$.

6 Conclusions

Based on the micro-block factorization introduced in [24] we have shown that a Bunch-Kaufman-Parlett like strategy with a priori known pivot structure can be employed for the explicit micro-block factorization of coefficients matrices from *regularized* saddle-point problems. This micro-block factorization induces a macro-block factorization $\mathbf{X} = \mathcal{L}_{\mathbf{X}} \mathcal{D}_{\mathbf{X}} \mathcal{L}_{\mathbf{X}}^T$ such that systems with the 3×3 macro-block matrices $\mathcal{L}_{\mathbf{X}}$ and $\mathcal{D}_{\mathbf{X}}$ can be solved efficiently. For the saddle-point case ($\mathbf{C} = \mathbf{0}$) the macro-block factorization is similar to that of [24] in the sense that the non-zero blocks of \mathcal{L} of [24, Lemma 4.1] have the same shape as the corresponding ones of $\mathcal{L}_{\mathbf{X}}$ in (28). If in addition $\text{diag}(\mathbf{B}_1) = \mathbf{I}_m$ then both matrices and in fact macro-block factorizations [24, Lemma 4.1] and (28) are identical. For systems with coupled physics an extension to a k by k micro-block factorization with $k > 2$ is straightforward. In addition to using the presented exact factorization as is, one can use it as a basis for the construction of implicit-factorization and other preconditioners.

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