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Some results on determinants and inverses of nonsingular pentadiagonal matrices

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Abstract

A block matrix analysis is proposed to justify, and modify, a known algorithm for computing in $O(n)$ time the determinant of a nonsingular $n \times n$ pentadiagonal matrix ($n \geq 6$) having nonzero entries on its second subdiagonal. Also, we describe a procedure for computing the inverse matrix with acceptable accuracy in $O(n^2)$ time. In the general nonsingular case, for $n \geq 5$, proper decompositions of the pentadiagonal matrix, as a product of two structured matrices, allow us to obtain both the determinant and the inverse matrix by exploiting low rank structures.

Keywords: Computational complexity, determinant, inverse matrix, pentadiagonal matrix, structured matrix.
2000 MSC: 15A09, 15A15, 15A23, 15A33, 65F05

1. Introduction

A nonsingular $n \times n$ matrix $\mathbf{P} = \{p_{ij}\}_{1 \leq i,j \leq n}$ is pentadiagonal if $p_{i,j} = 0$ for $|i - j| > 2$. These play an important role in contemporary numerical analysis. They arise frequently in numerical methods for solving ordinary and partial differential equations, interpolation schemes, and spline problems, [1]. Also, pentadiagonal matrices appear in fine approximations of second order derivatives, and in boundary value problems involving fourth order

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derivatives. Gaussian methods with partial pivoting are usually used for the inversion of such matrices. However, these methods can destroy the low rank structure and sparsity of pentadiagonal matrices; e.g. by row-interchange operations. Therefore, specialized techniques adapted to the low rank structure of pentadiagonal matrices are of interest.

Some specific parallel and sequential algorithms for the inversion of pentadiagonal matrices are already known. A recursive procedure for calculating in $O(n^2)$ time the inverse matrix $\mathbf{P}^{-1}$ of a pentadiagonal matrix $\mathbf{P}$ having nonzero entries on its second superdiagonal, $p_{i,j} \neq 0$ for $j - i = 2$, was given in [2]. In [3] there was proposed a different sequential procedure, having computational complexity $O(n^2)$, for pentadiagonal matrices having an LU (Doolittle) factorization.

Fast numerical algorithms for computing the determinants of pentadiagonal matrices are also needed to test efficiently for the existence of unique solutions of partial differential equations, and for solving the inverse problem of constructing symmetric pentadiagonal Toeplitz matrices. Some methods having complexity $O(n)$ have been obtained; see e.g. [4, 5, 6, 7, 8]. Building upon such results, in Section 2 we introduce a block matrix analysis to justify, in terms of matrix cofactors, the algorithm given in [6] for computing with complexity $O(n)$ the determinant, $\det \mathbf{P}$, of a pentadiagonal matrix having nonzero entries on its second subdiagonal. This kind of matrix is currently used in numerical methods. Since it is not hard to do, we find it convenient subsequently to adapt this algorithm to compute in $O(n^2)$ time the entire inverse matrix $\mathbf{P}^{-1}$, up to an acceptable accuracy. Analogous results can also be obtained for pentadiagonal matrices with nonzero entries on their second superdiagonals.

A specific procedure for computing both the determinant and the inverse of any nonsingular pentadiagonal matrix $\mathbf{P}$, taking advantage of its low rank structure, with no further conditions on its entries, remains an open question. In Section 3 we propose factorizations appropriate for the general nonsingular case where the pentadiagonal matrix $\mathbf{P}$ is decomposable as a product of two structured matrices; e.g. upper Hessenberg matrices (see also [9]). This enables us to exploit the low rank structure of (sparse) structured matrices, including triangular, tridiagonal, and Hessenberg matrices, to compute both the determinant, $\det \mathbf{P}$, and the inverse $\mathbf{P}^{-1}$. Illustrative comparisons, examples, and remarks are also presented.

2. Pentadiagonal matrices having nonzero entries on their second subdiagonals.

For an $n \times n$ ($n \geq 6$) nonsingular pentadiagonal matrix with nonzero entries on its second subdiagonal we assume the 2×2 block structure,

$$\mathbf{P} = \left(\begin{array}{c|c} \mathbf{P}_{11} & \mathbf{0}_2 \\ \hline \mathbf{U} & \mathbf{P}_{22} \end{array} \right). \tag{1}$$

The submatrices $\mathbf{P}_{11}$ and $\mathbf{P}_{22}$ have dimensions $2 \times n-2$ and $n-2 \times 2$, respectively. The matrix $\mathbf{0}_2$ is the 2×2 zero matrix. The $n-2 \times n-2$ nonsingular matrix $\mathbf{U}$ is upper triangular. The transposed partition,

$$\mathbf{P}^{-1} = \left(\begin{array}{c|c} -\mathbf{U}^{-1}\mathbf{P}_{22}\mathbf{M}_{21} & \mathbf{U}^{-1} + \mathbf{U}^{-1}\mathbf{P}_{22}\mathbf{M}_{21}\mathbf{P}_{11}\mathbf{U}^{-1} \\ \hline \mathbf{M}_{21} & -\mathbf{M}_{21}\mathbf{P}_{11}\mathbf{U}^{-1} \end{array} \right), \tag{2}$$

of its inverse is well known; see e.g. [10]. Here, $\mathbf{M}_{21} = \frac{1}{\det \mathbf{P}} \begin{pmatrix} C_{1,n-1} & C_{2,n-1} \\ C_{1,n} & C_{2,n} \end{pmatrix}$ is calculated using the classical Cayley cofactor formula for the inverse. The $C_{i,j}$ are cofactors of $\mathbf{P}$. Therefore, the inverse matrix

$$\mathbf{P}^{-1} = \begin{pmatrix} -\mathbf{U}^{-1}\mathbf{P}_{22} \\ \mathbf{I}_2 \end{pmatrix} \mathbf{M}_{21} \begin{pmatrix} \mathbf{I}_2 & -\mathbf{P}_{11}\mathbf{U}^{-1} \end{pmatrix} + \left(\begin{array}{c|c} \mathbf{0}_{n,2} & \mathbf{U}^{-1} \\ \hline \mathbf{0}_2 & \mathbf{0}_{2,n} \end{array} \right), \tag{3}$$

can be seen as a rank two perturbation of a strictly upper triangular matrix, [10]. All the information required for the inversion of $\mathbf{P}$ is contained in the submatrices $\mathbf{M}_{21}$ and $\mathbf{U}^{-1}$. As a result, we can calculate $\mathbf{P}^{-1}$ using simple matrix products as in (3).

2.1. Computing the determinant in $O(n)$ time

A compact expression for calculating the determinant of a nonsingular pentadiagonal matrix having nonzero entries on its second superdiagonal was given in [6]. It also applies to a matrix having nonzero entries on its second subdiagonal. A sequential algorithm for computing $\det \mathbf{P}$ with complexity $O(n)$ was also given. In order to justify, in terms of a computation using matrix cofactors, the formula for $\det \mathbf{P}$ given in [6], we introduce a second pentadiagonal matrix, $\mathbf{P}^*$, associated with $\mathbf{P}$ and having ones on its second subdiagonal. A variant of this related algorithm, together with (3), allows us to compute the full inverse matrix $\mathbf{P}^{-1}$.

Proposition 1. *Let* $\mathbf{P}$ *be an* $n\times n$ $(n \geq 6)$ *nonsingular pentadiagonal matrix having nonzero entries on its second subdiagonal. With* $\mathbf{P}$ *we associate the matrix* $\mathbf{P}^* = \mathbf{P}\cdot \mathbf{diag}\left(\frac{1}{p_{31}}, \frac{1}{p_{42}}, \cdots, \frac{1}{p_{n,n-2}}, 1, 1\right)$. *The determinant of* $\mathbf{P}$ *is given by*

$$\det \mathbf{P} = \left(\prod_{k=1}^{n-2} p_{k+2,k}\right) \det \begin{pmatrix} C^*_{1,n-1} & C^*_{2,n-1} \\ C^*_{1n} & C^*_{2n} \end{pmatrix}, \tag{4}$$

where the C^*_{ji} *are cofactors of the matrix* $\mathbf{P}^*$. *Moreover,* $\det \mathbf{P}$ *can be computed in* $O(n)$ *time.*

Proof. First, we note that $\det \mathbf{P} = \left(\prod_{k=1}^{n-2} p_{k+2,k}\right) \det \mathbf{P}^*$. Then we must demonstrate that $\det \mathbf{P}^* = \det \begin{pmatrix} C^*_{1,n-1} & C^*_{2,n-1} \\ C^*_{1n} & C^*_{2n} \end{pmatrix}$. The matrix $\mathbf{P}^*$ is pentadiagonal, with ones on its second subdiagonal.

Partitioning $\mathbf{P}^*$ as in (1) and $\mathbf{P}^{*-1}$ as in (2), we obtain a partition of the identity matrix $\mathbf{I}_n$, where $(\mathbf{P}^*\mathbf{P}^{*-1})_{11} = \mathbf{I}_2$. That is, $-\mathbf{P}^*_{11}\mathbf{U}^{*-1}\mathbf{P}_{22}\mathbf{M}^*_{21} = \mathbf{I}_2$. Since the matrix $\mathbf{U}^*$ in (1) is upper triangular with ones on its main diagonal, applying the nullity theorem [11], we conclude that the 2×2 matrix entry $\mathbf{M}^*_{21}$, in the transposed partition of $\mathbf{P}^{*-1}$, is nonsingular. Therefore, we have

$$\frac{1}{\det \mathbf{P}^*}\begin{pmatrix} C^*_{1,n-1} & C^*_{2,n-1} \\ C^*_{1n} & C^*_{2n} \end{pmatrix} = \mathbf{M}^*_{21} = \left(-\mathbf{P}^*_{11}\mathbf{U}^{*-1}\mathbf{P}_{22}\right)^{-1}. \tag{5}$$

Furthermore, we have $\det \mathbf{P}^* = \det \left(\begin{array}{c|c} \mathbf{P}^*_{11} & \mathbf{0}_2 \\ \hline \mathbf{U}^* & \mathbf{P}_{22} \end{array}\right)$. Although the combinatorial Laplace formula for computing determinants can be used to calculate $\det \mathbf{P}^*$, we give a simpler proof using the Schur complement of a matrix. Since

$$\left(\begin{array}{c|c} \mathbf{P}^*_{11} & \mathbf{0}_2 \\ \hline \mathbf{U}^* & \mathbf{P}_{22} \end{array}\right) = \left(\begin{array}{c|c} \mathbf{0} & \mathbf{I}_2 \\ \hline \mathbf{I}_{n-2} & \mathbf{0} \end{array}\right)\left(\begin{array}{c|c} \mathbf{U}^* & \mathbf{P}_{22} \\ \hline \mathbf{P}^*_{11} & \mathbf{0}_2 \end{array}\right),$$

we have $\det \mathbf{P}^* = \det \left(\begin{array}{c|c} \mathbf{U}^* & \mathbf{P}_{22} \\ \hline \mathbf{P}^*_{11} & \mathbf{0}_2 \end{array}\right)$. The calculation of this determinant is immediate using the Schur complement $\mathbf{P}^*/\mathbf{U}^* = \mathbf{0}_2 - \mathbf{P}^*_{11}\mathbf{U}^{*-1}\mathbf{P}_{22} = -\mathbf{P}^*_{11}\mathbf{U}^{*-1}\mathbf{P}_{22}$, of the matrix $\mathbf{P}^*$ with respect to $\mathbf{U}^*$. There results

$$\det \mathbf{P}^* = \det \mathbf{U}^* \det\left(-\mathbf{P}^*_{11}\mathbf{U}^{*-1}\mathbf{P}_{22}\right) = \det\left(\mathbf{P}^*_{11}\mathbf{U}^{*-1}\mathbf{P}_{22}\right). \tag{6}$$

Taking determinants in (5), and using (6), $\det \mathbf{P}^* = \det \begin{pmatrix} C^*_{1,n-1} & C^*_{2,n-1} \\ C^*_{1n} & C^*_{2n} \end{pmatrix}$.

Order	Matlab® ET	AHE ET	Matlab®	AHE	Sogabe
27	0.96e-04	0.68e-04	0	0	NaN
34	2.33e-04	1.22e-04	0	0	NaN
41	1.75e-04	0.90e-04	1	1	NaN
48	2.57e-04	1.22e-04	0	0	NaN
55	2.03e-04	0.89e-04	1	1	NaN

Table 1: Comparison of the time elapsed ET (in seconds) using the different algorithms for the computation of the determinant of a pentadiagonal matrix $\mathbf{P}$ with entries $p_{ij} = 1$, for $|i-j| \leq 2$, and $p_{ij} = 0$ otherwise.

The given cofactors of the matrix $\mathbf{P}^*$ are related with determinants of sparse upper Hessenberg matrices with ones on their subdiagonal entries. In addition, the involved cofactors are co-recurrent; i.e. they can be computed with the same 5-th order linear recurrence relation. Therefore, we can use a well-known recursive relation to compute such determinants with complexity $O(n)$. $\square$

Remark 1. *The determinantal formula for* $\mathbf{P}$ *can be derived directly using* (1) *and* $\mathbf{P}/\mathbf{U}$*, the Schur complement of* $\mathbf{P}$ *with respect to* $\mathbf{U}$*, i.e.* $\det \mathbf{P} = \det \mathbf{U} \det(\mathbf{P}/\mathbf{U}) = \left(\prod_{k=1}^{n-2} p_{k+2,k}\right) \det \begin{pmatrix} C_{1,n-1} & C_{2,n-1} \\ C_{1n} & C_{2n} \end{pmatrix}$*. Nevertheless, the equivalent expression* (4)*, with the cofactors of the matrix* $\mathbf{P}^*$*, is better for further computations.*

Given $\mathbf{P}$, we must compute $13n$ quotients and products (plus $6n$ sums) to obtain $\det \mathbf{P}$; $4n$ quotients to obtain $\mathbf{P}^*$, n products to obtain the entries on the second subdiagonal, and $8n$ products (plus $6n$ sums) to compute the cofactors from (4). The adapted Hadj-Elouafi algorithm (AHE) for computing $\det \mathbf{P}$ is described in Appendix A.

Example 1. *We compare the performance of the AHE algorithm with that of the built-in* Matlab® *function det() and the commonly used Sogabe algorithm [7], in the computation of the determinant of a pentadiagonal matrix* $\mathbf{P}$ *with entries* $p_{ij} = 1$*, for* $|i-j| \leq 2$*, and* $p_{ij} = 0$ *otherwise. The Sogabe algorithm breaks down because some principal submatrices are singular. The AHE procedure also works for singular pentadiagonal matrices with nonzero entries on their second subdiagonals. The numerical results are summarized in Table 1.*

Order	Matlab® ET	AHE ET	Sogabe ET	Value	Sogabe
27	1.04e-04	1.25e-04	1.17e-04	1.44e+12	NaN
34	1.71e-04	1.42e-04	0.61e-04	3.85e+13	3.85e+13
41	1.97e-04	1.59e-04	1.12e-04	3.50e+17	NaN
48	2.34e-04	1.61e-04	0.63e-04	1.71e+21	1.71e+21
55	2.96e-04	1.37e-04	0.61e-04	-4.83e+23	-4.83e+23

Table 2: Numerical values given by the algorithms for the times elapsed ET (in seconds) in the computation of the determinant of a pentadiagonal matrix $\mathbf{P}$ with random integer entries p_{ij} for $|i-j| \leq 2$ (and with nonzero entries on its second subdiagonal), and $p_{ij} = 0$ otherwise. Although the Sogabe algorithm is faster, it fails frequently.

Example 2. *We make another comparison by computing the determinant of a pentadiagonal matrix* $\mathbf{P}$*, with entries* p_{ij} *that are random integers in the interval* $[-3\ ,\ 3]$ *for* $|i-j| \leq 2$ *(and with nonzero entries on its second subdiagonal), and* $p_{ij} = 0$ *otherwise. The Sogabe algorithm is faster, but it fails frequently. The* Matlab® *and AHE algorithms always work, and yield equivalent outcomes. The numerical results are summarized in Table 2.*

2.2. Computing the inverse in $O(n^2)$ time

A fast recursive algorithm for computing with complexity $O(n^2)$ the inverse matrices of this kind of nonsingular pentadiagonal matrices was proposed in [2]. When the matrix size increases, the accuracy of such an algorithm might be inadequate because of the recurrence formulas involved; see e.g. [12].

We can propose an alternative procedure building a new recursive algorithm for obtaining $\mathbf{M}_{21}$ and $\mathbf{P}^*$ using the algorithm from Appendix A (which is based on Proposition 1). Then, we can compute the remaining entries of the inverse matrix via recurrence formulas, using a procedure similar to that used in [2]. Indeed, we calculate $\mathbf{M}_{21}$ and $\mathbf{P}^*$ in order to compute the first and second columns of the inverse matrix $\mathbf{P}^{-1}$ using recurrence formulas. The remaining columns are obtained in a recursive way, as in the algorithm in [2]. Nevertheless, this alternative procedure suffers from the same drawback regarding the accuracy of the outcomes as the algorithm from [2].

Example 3. *This difficulty is illustrated in Table 3 which records the mean values, over 100 trials, for the times elapsed and the norms related with*

Matrix order	Hadj-Elouafi Elapsed time	Proposed Elapsed time	Hadj-Elouafi $\lvert\lvert\mathbf{P}\cdot\mathbf{P}^{-1}-\mathbf{I}_n\rvert\rvert_2$	Proposed $\lvert\lvert\mathbf{P}\cdot\mathbf{P}^{-1}-\mathbf{I}_n\rvert\rvert_2$
24	1.69e-04	1.99e-04	1.46e-08	2.96e-07
30	1.70e-04	2.33e-04	1.73e-06	7.32e-07
36	2.28e-04	3.32e-04	1.76e-02	1.50e-05
42	2.28e-04	2.31e-04	1.10e-01	6.26e-04
48	2.44e-04	2.38e-04	1.54e-02	2.78e-02
54	2.89e-04	2.70e-04	4.32e+01	1.08e+00

Table 3: Mean values of the times elapsed (in seconds) and norms $||\mathbf{P}\cdot\mathbf{P}^{-1}-\mathbf{I}_n||_2$, over 100 trials, of the two procedures from Example 3 for inverting a pentadiagonal matrix $\mathbf{P}$ with random integer entries p_{ij} from the interval $[-2\ ,\ 3]$ for $|i-j|\leq 2$ (and with nonzero entries on its second subdiagonal), and $p_{ij}=0$ otherwise. Although both procedures are fast, the lack of accuracy is remarkable.

the largest singular value of the matrices $\mathbf{P}\cdot\mathbf{P}^{-1}-\mathbf{I}_n$, the matrix 2-norm $||\mathbf{P}\cdot\mathbf{P}^{-1}-\mathbf{I}_n||_2$. We have compared both the Hadj-Elouafi algorithm and the alternative procedure proposed above for the inversion of a pentadiagonal matrix $\mathbf{P}$ with random integer entries p_{ij} from the interval $[-2\ ,\ 3]$ for $|i-j|\leq 2$ (and with nonzero entries on its second subdiagonal), and $p_{ij}=0$ otherwise.

The procedure for computing $\det\mathbf{P}$ given in Appendix A, and justified in Proposition 1, can also be used to compute the submatrices $\mathbf{M}_{21}$ and $\mathbf{U}^{-1}$ in (3) in a more accurate way. Recall that such matrices provide complete information about the inverse $\mathbf{P}^{-1}$. It is not difficult to see that $\mathbf{M}_{21}=\frac{1}{\det\mathbf{P}}\begin{pmatrix} C_{1,n-1} & C_{2,n-1}\\ C_{1n} & C_{2n}\end{pmatrix}=\frac{1}{\det\mathbf{P}^*}\begin{pmatrix} C^*_{1,n-1} & C^*_{2,n-1}\\ C^*_{1n} & C^*_{2n}\end{pmatrix}$. Consequently, we can compute $\mathbf{M}_{21}$ with complexity $O(n)$ by using the algorithm from Appendix A. In addition, we can obtain the unit upper triangular submatrix $\mathbf{P}^*(3:n,1:n-2)$ (consisting of the rows $3,4,\cdots,n$ and the columns $1,2,\cdots,n-2$ of $\mathbf{P}^*$) using the same algorithm. This sparse matrix is useful for computing the matrix $\mathbf{U}^{-1}$ by forward substitution; see e.g. [13, 14]. We can compute $\mathbf{U}^{-1}$ in $O(n^2)$ time. That is, given that the matrix $\mathbf{P}^*(3:n,1:n-2)$ has been computed in O(n) time, the main cost in determining $\mathbf{U}^{-1}$ with enhanced accuracy is $2n^2+O(n)$ flop counts for the products, plus $\frac{3}{2}n^2+O(n)$ flop counts for the sums. Therefore, the inverse matrix can be computed from $\mathbf{M}_{21}$ and $\mathbf{U}^{-1}$ in $O(n^2)$ time using (3). However, when the size of the matrix grows, the accumulated round-off errors of the products of matrices in (3)

Order	24	30	36	42	48	54
ET	1.71e-04	1.83e-04	2.26e-04	2.15e-04	2.66e-04	2.77e-04
Norm	9.05e-13	3.33e-12	5.76e-11	1.38e-10	1.34e-09	6.53e-08

Table 4: Mean values of the time elapsed ET (in seconds) and norm $= ||\mathbf{U}\cdot\mathbf{U}^{-1} - \mathbf{I}_{n-2}||_2$, over 100 trials, using the algorithm from Appendix B to obtain more accurate information about the full inverse of a random pentadiagonal matrix $\mathbf{P}$, as in Example 3.

need to be controlled; see e.g. [12].

Example 4. *The performance of the algorithm from Appendix B is recorded in Table 4, which gives us the mean values of the time elapsed (in seconds) and norm* $||\mathbf{U}\cdot\mathbf{U}^{-1} - \mathbf{I}_{n-2}||_2$, *over 100 trials, in the computation of the inverse of a pentadiagonal matrix, as in Example 3. The outcomes are now more accurate.*

Remark 2. *The procedure detailed in Appendix B for computing the matrices* $\mathbf{M}_{21}$ *and* $\mathbf{U}^{-1}$ *helps explain the motivation for introducing the AHE algorithm. The sparse matrix* $\mathbf{P}^*(3:n, 1:n-2)$ *is unit upper triangular. Hence, the matrix* $\mathbf{U}^{-1}$ *is obtained by a simple forward substitution scheme.*

3. Nonsingular pentadiagonal matrices. The general setting.

In a general situation specific procedures are required to compute the inverse of a nonsingular pentadiagonal matrix $\mathbf{P}$ for which no further conditions are imposed on its entries, e.g. when the low rank structure of the pentadiagonal matrix is broken by using LU methods with row-interchange operations. Such a general procedure for computing both the determinant and the inverse of a general nonsingular pentadiagonal matrix $\mathbf{P}$ is not yet available. We propose here appropriate factorizations of $\mathbf{P}$ as a product of two nonsingular structured matrices with ranks lower than $\mathbf{P}$. Such decompositions allow us to use well-known methods for preserving low rank structures in the inversion of the involved matrices; see e.g. [15, 16, 17].

The subdiagonal rank of an $n \times n$ matrix $\mathbf{M}$ is defined as $sr(\mathbf{M}) = \max \operatorname{rank} \{\mathbf{M}(i:n\ ,\ 1:i-1) : i = 2, 3, \cdots, n\}$; see [9] and references therein. In an analogous way, the superdiagonal rank of an $n \times n$ matrix $\mathbf{M}$ is defined as $Sr(\mathbf{M}) = \max \operatorname{rank} \{\mathbf{M}(1:i\ ,\ i+1:n) : i = 1, 2, \cdots, n-1\}$. For a pentadiagonal matrix $\mathbf{P}$ the subdiagonal rank $sr(\mathbf{P})$ is at most 2. The case

$sr(\mathbf{P}) = 1$ implies that $\mathbf{P}$ is also a generalized Hessenberg matrix. This case has been considered in [9]. The structured matrices involved in the factorizations of $\mathbf{P}$ will be chosen in such a way that their subdiagonal ranks are 1. This is also true for the transposed factorization of the inverse matrix $\mathbf{P}^{-1}$, [9].

Furthermore, we assume that a general $n \times n$ $(n \geq 5)$ nonsingular pentadiagonal matrix $\mathbf{P}$ has the 2×2 block matrix partition

$$\mathbf{P} = \left(\begin{array}{c|c} \mathbf{R} & 0 \\ \hline \mathbf{H} & \mathbf{C} \end{array} \right). \tag{7}$$

Here $\mathbf{R}$ is a $1 \times n-1$ row matrix, $\mathbf{C}$ is an $n-1 \times 1$ column matrix, and the $n-1 \times n-1$ matrix $\mathbf{H} = \mathbf{P}(2:n, 1:n-1)$ is upper Hessenberg.

3.1. Submatrix $\mathbf{H}$ *having an* $L_H U_H$ *(Doolittle) factorization*

Before the introduction of the general case, we consider the important special case when the submatrix $\mathbf{H}$ in (7) has an $L_H U_H$ factorization.

Proposition 2. *Let* $\mathbf{P}$ *be an* $n \times n$ $(n \geq 5)$ *nonsingular pentadiagonal matrix. We assume that, in the block partition* (7)*, the submatrix* $\mathbf{H}$ *has an* $L_H U_H$ *factorization. Then, there exists a decomposition of* $\mathbf{P}$ *of the form*

$$\mathbf{P} = \mathbf{L}\mathbf{H}_U = \left(\begin{array}{c|c} 1 & \mathbf{0}_{n-1}^T \\ \hline \mathbf{0}_{n-1} & \mathbf{L_H} \end{array} \right) \left(\begin{array}{c|c} \mathbf{R} & 0 \\ \hline \mathbf{U_H} & \mathbf{L_H}^{-1}\mathbf{C} \end{array} \right), \tag{8}$$

with $\mathbf{L}$ *a unit lower triangular matrix such that* $sr(\mathbf{L}) = 1$*, and* $\mathbf{H}_U$ *an upper Hessenberg matrix with* $sr(\mathbf{H}_U) = 1$*.*

Proof. With the given assumptions, the existence of the factorization (8) is immediate. If we take the product of matrices, we obtain the block matrix $\mathbf{P}$ as in (7). Note that the $L_H U_H$ factorization of the sparse upper Hessenberg matrix $\mathbf{H}$ can be obtained trivially.

The matrices $\mathbf{L}$ and $\mathbf{H}_U$ are nonsingular because we assume that the matrix $\mathbf{P}$ is nonsingular. Since $\mathbf{H}_U$ is upper Hessenberg, $sr(\mathbf{H}_U) = 1$. Furthermore, it is not difficult to check that $sr(\mathbf{L}) = sr(\mathbf{L_H}) = sr(\mathbf{H}) = 1$. $\square$

When the Hessenberg submatrix $\mathbf{H}$ is nonsingular, the $L_H U_H$ factorization has a unit lower triangular matrix $\mathbf{L_H}$. The matrix $\mathbf{L}$ is also unit and the upper Hessenberg matrix $\mathbf{H}_U$ is unreduced; i.e. with nonzero entries on its first subdiagonal. When $\mathbf{H}$ is singular, with an $L_H U_H$ factorization that need not be unique, the lower triangular matrix $\mathbf{L_H}$ can be taken to be nonsingular, with unit determinant. Hence, the matrix $\mathbf{L}$ is also unit, but now the matrix $\mathbf{H}_U$ is reduced.

3.1.1. Nonsingular submatrix $\mathbf{H}$

If the submatrix $\mathbf{H}$ in (7) is nonsingular and has nonzero entries on its main diagonal, we can obtain a factorization equivalent to (8), without using the $L_H U_H$ factorization of $\mathbf{H}$. Indeed, we define $\mathbf{H} = \mathbf{L}_H^* \mathbf{U}_H^*$, where $\mathbf{L}_H^*$ is lower triangular with diagonal and subdiagonal entries equal to those of $\mathbf{H}$. The matrix $\mathbf{U}_H^*$ is upper triangular, for $\mathbf{U}_H^* = \mathbf{L}_H^{*-1}\mathbf{H}$. Here the inverse matrix $\mathbf{L}_H^{*-1}$ is easy to compute.

Example 5. *Suppose given the pentadiagonal matrix*

$$\mathbf{P} = \left(\begin{array}{cccc|c} 1 & 1 & 0 & 0 & 0 \\ \hline 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & -1 & 1 & 1 \end{array}\right) = \left(\begin{array}{c|cccc} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{array}\right) \left(\begin{array}{cccc|c} 1 & 1 & 0 & 0 & 0 \\ \hline 1 & 1 & 1 & 1 & 0 \\ 0 & 2 & 2 & 2 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 2 & 2 \end{array}\right),$$

which admits no LU factorization. Here, the submatrix $\mathbf{H}$ *in* (7) *is nonsingular, and has an* $L_H U_H$ *factorization. Instead of the* $L_H U_H$ *factorization of* $\mathbf{H}$*, we have used the matrices defined above. The determinant is* $\det \mathbf{P} = \det \mathbf{H}_U = 4$*. The transposed factorization of the inverse matrix* $\mathbf{P}^{-1}$ *is*

$$\mathbf{P}^{-1} = \left(\begin{array}{cccc|c} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 \\ \hline \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 & -\frac{1}{2} \\ -1 & 1 & 0 & -1 & \frac{1}{2} \\ 1 & -1 & 0 & 1 & 0 \end{array}\right) \left(\begin{array}{c|cccc} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{array}\right).$$

Remark 3. *When the nonsingular submatrix* $\mathbf{H}$ *in* (7) *has nonzero entries on its main diagonal, the* $L_H U_H$ *factorization of* $\mathbf{H}$ *is crucial for the existence of a factorization of the pentadiagonal matrix* $\mathbf{P} = \mathbf{L}\mathbf{H}_U$*. The reader can easily check that the matrix* $\mathbf{P} = \left(\begin{array}{cccc|c} 1 & 1 & 0 & 0 & 0 \\ \hline 1 & 1 & 1 & -1 & 0 \\ 1 & 1 & 2 & -1 & 1 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & -1 \end{array}\right)$ *has neither a factorization as in Example 5 nor as in Proposition* 2*, because the nonsingular submatrix* $\mathbf{H}$ *has no* $L_H U_H$ *factorization.*

3.1.2. Singular submatrix $\mathbf{H}$

An $n \times n$ matrix $\mathbf{M}$ in the algebra of square matrices, $M_n(\mathbb{K})$ ($\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$), has a unique LU factorization if and only if its $k \times k$ principal submatrices have full rank; $k = 1, 2, \cdots, n-1$. Applying this fact when the submatrix $\mathbf{H}$ in (7) is singular, it follows that its $L_H U_H$ factorization (if it exists) is not necessarily unique. Furthermore, when the singular submatrix $\mathbf{H}$ has a unique $L_H U_H$ factorization, we cannot decompose $\mathbf{H}$ as a product $\mathbf{H} = \mathbf{L}_H^* \mathbf{U}_H^*$ because $\mathbf{H}$ does not have full rank. Hence, if $\mathbf{H}$ is singular, with an $L_H U_H$ factorization, we use the decomposition (8).

Example 6.

$$\mathbf{P} = \left(\begin{array}{cccc|c} 1 & 1 & 0 & 0 & 0 \\ \hline 1 & 1 & 1 & 0 & 0 \\ 0 & 2 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 2 \\ 0 & 0 & 1 & 1 & 1 \end{array}\right) = \left(\begin{array}{c|cccc} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 1 & 0 \\ 0 & 0 & 0 & 2 & 1 \end{array}\right) \left(\begin{array}{cccc|c} 1 & 1 & 0 & 0 & 0 \\ \hline 1 & 1 & 1 & 0 & 0 \\ 0 & 2 & 1 & 1 & 1 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{3}{2} \\ 0 & 0 & 0 & 0 & -2 \end{array}\right).$$

Note that we cannot obtain a factorization, with $\mathbf{H} = \mathbf{L}_H^* \mathbf{U}_H^*$ *as in Example 5.*

3.2. The general setting

When the partitioned pentadiagonal matrix $\mathbf{P}$ from (7) does not admit the decomposition (8), its submatrix $\mathbf{H}$ has rank deficiency; i.e. $\mathbf{H}$ does not satisfy the known $n-1$ conditions, $rank\,\{\mathbf{H}(1:i, 1:i)\} + i \geq rank\,\{\mathbf{H}(1:i, 1:n-1)\} + rank\,\{\mathbf{H}(1:n-1, 1:i)\}$, and $i = 1, 2, \cdots, n-1$. That is, $\mathbf{H}$ has no $L_H U_H$ factorization. To overcome this nontrivial difficulty, and taking into account that $\mathbf{H}$ is upper Hessenberg, we propose a general factorization $\mathbf{H} = \mathbf{H}^* \mathbf{U}^*$, where the nonsingular matrix $\mathbf{H}^*$ is upper Hessenberg, and the matrix $\mathbf{U}^*$ is upper triangular. This factorization covers all possible rank deficiency situations and gives rise to the following general decomposition (as a product of two matrices with subdiagonal rank 1) for a fully general pentadiagonal matrix.

Theorem 1. *Let* $\mathbf{P}$ *be a general* $n \times n$ $(n \geq 5)$ *nonsingular pentadiagonal matrix partitioned as in* (7)*. Then,* $\mathbf{P}$ *has a decomposition*

$$\mathbf{P} = \left(\begin{array}{c|c} 1 & \mathbf{0}_{n-1}^T \\ \hline \mathbf{0}_{n-1} & \mathbf{H}^* \end{array}\right) \left(\begin{array}{c|c} \mathbf{R} & 0 \\ \hline \mathbf{U}^* & \mathbf{H}^{*-1}\mathbf{C} \end{array}\right), \tag{9}$$

as a product of two upper Hessenberg matrices, where

a) $\mathbf{H}^* = \mathbf{H}$ *and* $\mathbf{U}^* = \mathbf{I}_{n-1}$*, for nonsingular* $\mathbf{H}$*.*

b) $\mathbf{H}^*\mathbf{U}^* = \mathbf{H}$*, for singular* $\mathbf{H}$ *.*

Proof. In case a), when the submatrix $\mathbf{H}$ is nonsingular, the claim is trivial. In case b), when $\mathbf{H}$ is singular, the existence of such a factorization follows from the fact that we can find a nonsingular upper Hessenberg matrix $\mathbf{H}^*$, with the same subdiagonal and diagonal entries than $\mathbf{H}$. The upper half of $\mathbf{H}^*$ can be chosen in such a way as to give the factorization $\mathbf{H}^*\mathbf{U}^* = \mathbf{H}$. The upper triangular matrix $\mathbf{U}^* = \mathbf{H}^{*-1}\mathbf{H}$ is singular. The subdiagonal rank of the upper Hessenberg matrix is obviously 1. □

Although alternative procedures have been proposed, this factorization also applies to a nonsingular pentadiagonal matrix having nonzero entries on its second subdiagonal, or having a submatrix $\mathbf{H}$ admitting an $L_H U_H$ factorization.

3.2.1. Nonsingular submatrix $\mathbf{H}$

The factorization for the pentadiagonal matrix $\mathbf{P}$ given in (9) when the matrix $\mathbf{H} = \mathbf{P}(2:n, 1:n-1)$ is nonsingular (case a)) yields

$$\mathbf{P} = \left(\begin{array}{c|c} 1 & \mathbf{0}_{n-1}^T \\ \hline \mathbf{0}_{n-1} & \mathbf{H} \end{array}\right)\left(\begin{array}{c|c} \mathbf{R} & 0 \\ \hline \mathbf{I}_{n-1} & \mathbf{H}^{-1}\mathbf{C} \end{array}\right). \tag{10}$$

For convenience, we assume that $\mathbf{H}$ is reduced; i.e. $\mathbf{H}$ has some null entries on its subdiagonal. The method is also applicable when $\mathbf{H}$ is unreduced, but see also the methods described in Section 2. The determinant of the Hessenberg matrix on the left of (10) is $\det \mathbf{H}$. For computing the determinant of the Hessenberg matrix on the right of (10) we define a column vector, $\mathbf{X} = \mathbf{H}^{-1}\mathbf{C}$, of size $n-1$. We obtain the value $(-1)^n(r_1x_1+r_2x_2+r_3x_3)$, e.g. by expanding the determinant along the last column of the matrix. Therefore, we have

$$\det \mathbf{P} = (-1)^n \det \mathbf{H} \cdot (r_1x_1 + r_2x_2 + r_3x_3)\,. \tag{11}$$

There is no difficulty in obtaining the transposed factorization

$$\mathbf{P}^{-1} = \left(\begin{array}{c|c} \alpha\mathbf{X} & \mathbf{I}_{n-1} - \alpha\mathbf{X}\mathbf{R} \\ \hline -\alpha & \alpha\mathbf{R} \end{array}\right)\left(\begin{array}{c|c} 1 & \mathbf{0}_{n-1}^T \\ \hline \mathbf{0}_{n-1} & \mathbf{H}^{-1} \end{array}\right), \tag{12}$$

for the inverse matrix, where we defined $\alpha = \frac{1}{r_1x_1+r_2x_2+r_3x_3}$.

A simple matrix product allows us to decompose the inverse matrix

$$\mathbf{P}^{-1} = -\alpha \begin{pmatrix} -\mathbf{H}^{-1}\mathbf{C} \\ 1 \end{pmatrix} \begin{pmatrix} 1 & -\mathbf{R}\mathbf{H}^{-1} \end{pmatrix} + \left(\begin{array}{c|c} \mathbf{0}_{n-1} & \mathbf{H}^{-1} \\ \hline 0 & \mathbf{0}_{n-1}^T \end{array}\right) \tag{13}$$

as a rank one perturbation of a (singular) block upper triangular matrix; see also (3). In this way we obtain the needed information about the inverse matrix $\mathbf{P}^{-1}$ by inverting the (sparse) upper Hessenberg matrix $\mathbf{H}$.

Example 7. *We illustrate the preceding with the pentadiagonal matrix* $\mathbf{P}$ *admitting no LU factorization, described in Remark 3. Its submatrix* $\mathbf{H}$ *is nonsingular and admits no* $L_H U_H$ *factorization. We have* $\alpha = -\frac{1}{2}$. *Its determinant is* $\det \mathbf{P} = (-1)^5 \cdot \det \mathbf{H} \cdot (-2) = -2$, *by* (11). *The decomposition* (13) *for the inverse matrix yields*

$$\mathbf{P}^{-1} = \frac{1}{2} \left(\begin{array}{c} 3 \\ -1 \\ -1 \\ 1 \\ \hline 1 \end{array}\right) \left(\begin{array}{c|cccc} 1 & -2 & 1 & 0 & -1 \end{array}\right) + \left(\begin{array}{c|cccc} 0 & 1 & 0 & -1 & 2 \\ 0 & 1 & -1 & 1 & -1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 & 0 \end{array}\right).$$

3.2.2. Singular submatrix $\mathbf{H}$

When the submatrix $\mathbf{H} = \mathbf{P}(2:n, 1:n-1)$ is singular, the factorization of the pentadiagonal matrix $\mathbf{P}$ from (9) (case b)) yields

$$\mathbf{P} = \left(\begin{array}{c|c} 1 & \mathbf{0}_{n-1}^T \\ \hline \mathbf{0}_{n-1} & \mathbf{H}^* \end{array}\right) \left(\begin{array}{c|c} \mathbf{R} & 0 \\ \hline \mathbf{U}^* & \mathbf{H}^{*-1}\mathbf{C} \end{array}\right). \tag{14}$$

The upper Hessenberg matrix $\mathbf{H}^*$ can be taken to be nonsingular, with the same subdiagonal and diagonal entries as $\mathbf{H}$. Its related upper triangular matrix $\mathbf{U}^*$ must be singular. Note that in general such a factorization is not unique. Sometimes the matrix $\mathbf{H}^*$ can be taken tridiagonal. Then as a rule, we include in the superdiagonal as many zeros as possible, while preserving the nonsingularity of the matrix $\mathbf{H}^*$. This simplifies the inversion of the tridiagonal matrix; see e.g. [17].

The matrices involved in the factorization (14) are block (diagonal and upper triangular) matrices, with triangular, tridiagonal, or Hessenberg matrix entries on their diagonals. The determinants of such structured matrices are easily obtained using well-known recurrence relations. Consequently, $\det \mathbf{P}$ can be computed as a product of determinants.

Remark 4. *In the general case, the nonsingular submatrix* $\mathbf{H}^*$ *must be taken to be upper Hessenberg. This necessity is related to the superdiagonal rank of the submatrix* $\mathbf{H}$, $Sr(\mathbf{H})$, *as we observe in the next example.*

Example 8. *First, we illustrate* (14) *by factoring a pentadiagonal matrix* $\mathbf{P}$ *admitting no LU factorization,*

$$\mathbf{P} = \left(\begin{array}{cccc|c} 2 & 1 & 1 & 0 & 0 \\ \hline 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 \\ 0 & 0 & 1 & 1 & 1 \end{array}\right) = \left(\begin{array}{c|cc|cc} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{array}\right) \left(\begin{array}{cccc|c} 2 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 2 \\ \hline 0 & 0 & 0 & 0 & -1 \end{array}\right).$$

Note that $Sr(\mathbf{H}) = 2$. *The nonsingular matrix* $\mathbf{H}^*$ *can be taken to be tridiagonal and reduced. We have* $\det \mathbf{P} = (1\cdot(-1)\cdot 1)\,(2\cdot(-1)) = 2$ *using the block diagonal entries. The transposed factorization for the inverse* $\mathbf{P}^{-1}$ *is straightforward. However, for the pentadiagonal matrix,*

$$\mathbf{P} = \left(\begin{array}{cccc|c} 2 & 1 & 1 & 0 & 0 \\ \hline 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 \end{array}\right) = \left(\begin{array}{c|cccc} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \end{array}\right) \left(\begin{array}{cccc|c} 2 & 1 & 1 & 0 & 0 \\ \hline 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right),$$

with $Sr(\mathbf{H}) = 1$, *the factorization* (14) *does not admit a nonsingular tridiagonal matrix on the left. We can compute easily both* $\det \mathbf{P}$ *and the transposed factorization of the inverse matrix* $\mathbf{P}^{-1}$ *by exploiting low rank structures.*

Remark 5. *Various procedures can be proposed for computing the determinants and inverse matrices of nonsingular pentadiagonal matrices having factorizations as in* (8) *or* (9). *This can be useful in the inversion of pentadiagonal matrices admitting no LU factorization, where row-interchange operations are compulsory and the low rank structure of the pentadiagonal matrices is destroyed.*

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Appendix A. The adapted Hadj-Elouafi algorithm

Algorithm 1. The adapted Hadj-Elouafi algorithm, AHE, for computing the determinant of a pentadiagonal matrix $\mathbf{P}$ having nonzero entries on its second subdiagonal.

Input: The matrix $\mathbf{P}$ and its order n.

Output: The determinant, $\det \mathbf{P}$.

Step 1: Obtain $\mathbf{P}^*$ and the product $= \left(\prod_{k=1}^{n-2} p_{k+2,k}\right)$.

product = 1;

for $j = 1 : n-2$
product $= p_{j+2,j} \cdot$product;
for $i = j-2 : j+1$
$p^*_{ij} = \frac{p_{ij}}{p_{j+2,j}}$;
end
end

Step 2: Obtain the involved cofactors and $\det \mathbf{P}^*$ using recurrences.

$C^*_{0,1} = 1$; $C^*_{0,2} = 1$; $C^*_{1,1} = p^*_{21}$; $C^*_{1,2} = p^*_{11}$;

Compute $C^*_{j,1}$ and $C^*_{j,2}$, $2 \leq j \leq 4$, using recurrences.

for $j = 5 : n-2$

$C^*_{j,1} = p^*_{j+1,j} \cdot C^*_{j-1,1} - p^*_{jj} \cdot C^*_{j-2,1} + p^*_{j-1,j} \cdot C^*_{j-3,1} - p^*_{j-2,j} \cdot C^*_{j-4,1}$;

$C^*_{j,2} = p^*_{j+1,j} \cdot C^*_{j-1,2} - p^*_{jj} \cdot C^*_{j-2,2} + p^*_{j-1,j} \cdot C^*_{j-3,2} - p^*_{j-2,j} \cdot C^*_{j-4,2}$;

end

Compute $C^*_{j,1}$ and $C^*_{j,2}$, $n-1 \leq j \leq n$;

$\det \mathbf{P}^* = C^*_{n-1,1} \cdot C^*_{n,2} - C^*_{n,1} \cdot C^*_{n-1,2}$;

Step 3: Obtain $\det \mathbf{P}$ using expression (4).

$\det \mathbf{P} = \text{product} \cdot \det \mathbf{P}^*$.

Appendix B. Algorithm for computing the matrices $\mathbf{M_{21}}$ and $\mathbf{U^{-1}}$.

Algorithm 2. To compute the matrices $\mathbf{M}_{21}$ and $\mathbf{U}^{-1}$ from (3). These matrices supply the information necessary for inverting a nonsingular pentadiagonal matrix $\mathbf{P}$ having nonzero entries on its second subdiagonal.

Input: The matrix $\mathbf{P}$ and its order n.

Output: The matrices $\mathbf{M}_{21}$ and $\mathbf{U}^{-1}$.

Step 1: Compute the matrices $\mathbf{M}_{21}$ and $\mathbf{P}^*(3:n, 1:n-2)$.

Step 2: Compute the matrix $\mathbf{U}^{-1}$ using a forward substitution scheme.

for $i = 1 : n-2$

$u_{ii}^{-1} = p_{i+2,i}^*$;

end

$u_{12}^{-1} = -u_{11}^{-1} \cdot p_{32}^*$;

$u_{13}^{-1} = -u_{11}^{-1} \cdot p_{33}^* - u_{12}^{-1} \cdot p_{43}^*$; $\quad u_{23}^{-1} = -u_{21}^{-1} \cdot p_{33}^* - u_{22}^{-1} \cdot p_{43}^*$;

for $i = 1 : 3$

$u_{i4}^{-1} = -u_{i1}^{-1} \cdot p_{34}^* - u_{i2}^{-1} \cdot p_{44}^* - u_{i3}^{-1} \cdot p_{54}^*$;

end

for $j = 5 : n-2$, for $i = 1 : j-1$, $u_{ij}^{-1} = 0$;

for $k = j-4 : j-1$

$u_{ij}^{-1} = u_{i,k}^{-1} \cdot p_{k+2,j}^* + u_{ij}^{-1}$;

end, $u_{ij}^{-1} = -u_{ij}^{-1}$;

end, end

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