Relationship between the Inverses of a Matrix and a Submatrix

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Abstract. A simple and straightforward formula for computing the inverse of a submatrix in terms of the inverse of the original matrix is derived. General formulas for the inverse of submatrices of order $n-k$ as well as block submatrices are derived. The number of additions (or subtractions) and multiplications (or divisions) on the formula is calculated. A variety of numerical results are shown.

Keywords. Matrix inverse, submatrix, discrete Fourier transform.

1 Introduction

There are a number of situations in which the inverse of a matrix must be computed. For example, in statistics [17], where the inverse can provide important statistical information in certain matrix iterations arising in eigenvalue-related problems.

Direct methods for calculating the inverse of matrices include LU Decomposition, Cholesky Decomposition, and Gaussian Elimination [12, 17].

In Vandermonde matrices

$$V = V(\alpha_0, \dots, \alpha_n) = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ \alpha_0 & \alpha_1 & \cdots & \alpha_n \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_0^n & \alpha_1^n & \cdots & \alpha_n^n \end{pmatrix},$$

which arise in many approximation and interpolation problems, V is non-singular if scalars $\alpha_i,\ i = 0, \dots, n$ are different. The inverse of V can be calculated explicitly with $6n^2$ flops (see [17], p. 416). El-Mikkawy [11] provides an explicit expression for the inverse of generalized Vandermonde matrices by using elementary symmetric functions. Fourier matrices obtained from the Discrete Fourier Transform (DFT) are Vandermonde matrices with known inverses [12, 17].

Let A be a non-singular matrix and A^{-1} be its inverse. Sometimes, it is necessary to determine the inverse of an invertible submatrix of A. This situation is common in applied physics for superconductivity computations [15], photonic crystals [8, 21], metal-dielectric materials [25], and bianisotropic metamaterials [22].

In general, computation of the inverse of a submatrix from a matrix with the known inverse is not direct. Quite recently, Chang [9] provided a recursive method for calculating the inverse of submatrices located at the upper left corner of A.

In this paper, we aim to calculate the inverse of a non-singular submatrix in terms of the elements of the inverse of the original matrix. We compare the number of operations in our method with those of the Sherman-Morrison method and the LU Decomposition.

This problem is directly related to how to calculate the inverse of a perturbed matrix $(A + D)^{-1}$, where D is a perturbation matrix of A [10, 14, 19, 24]. This matrix inverse has been calculated in various disciplines with different applications, derived from the Sherman-Morrison formula [5, 23]:

$$(A - uv^T)^{-1} = A^{-1} + \frac{(A^{-1}u)(v^TA^{-1})}{1 - v^TA^{-1}u}, \tag{1}$$

where $u,\ v \in \mathbb{R}^n$ are column vectors, from the Sherman-Morrison-Woodbury formula [14, 16]:

$$[A - UV]^{-1} = A^{-1} + A^{-1}U\,(I - VA^{-1}U)^{-1}\,VA^{-1},$$

or from its block-partitioned matrix form [14]:

$$M^{-1} = \begin{pmatrix} A^{-1} + A^{-1}UC^{-1}VA^{-1} & -A^{-1}UC^{-1} \\ -C^{-1}VA^{-1} & C^{-1} \end{pmatrix}, \qquad (2)$$

where

$$M = \begin{pmatrix} A & U \\ V & D \end{pmatrix}, \qquad (3)$$

and $C = D - VA^{-1}U$ is the Schur complement of A.

Particularly, formula (2) has been applied by inverting a matrix with the enlargement method [13], which uses the same formula to express the inverse of a leading principal submatrix of order k in terms of a previously calculated submatrix of order $(k-1)$.

Applications of these formulas have been described in various papers. For example, Hager [14] discusses applications in statistics, networks, structural analysis, asymptotic analysis, optimization, and partial differential equations; Maponi [18] and Bru et al., [7] in solving linear systems of equations; Arsham, Grad, and Jaklič [4] in linear programming; Akgün, Garcelon, and Haftka [1] in structural reanalysis; and Alshehri [3] in the multi-period demand response management problem.

Now, we show a case where the perturbation matrix $A - uv^T$ can be used to solve the problem of calculating the inverse of an invertible submatrix of order $n-1$ of a known invertible matrix.

Let $A_{\bar{p};\bar{q}}$ be the submatrix obtained from A by eliminating the $p-\mathrm{th}$ row and $q-\mathrm{th}$ column. We state $A - uv^T$ by defining $u = A_q - e_p$, where A_q is the $q-\mathrm{th}$ column vector of A, $e_p \in \mathbb{R}^n$ is the $p-\mathrm{th}$ canonical column vector, and $v = e_q$ is the $q-\mathrm{th}$ canonical column vector. With these definitions, $A - uv^T$ is equal to A except in its $q-\mathrm{th}$ column, which is equal to e_p. By applying the Sherman-Morrison formula to calculate $(A - uv^T)^{-1}$, then $\left(A_{\bar{p};\bar{q}}\right)^{-1}$ is obtained by eliminating the $q-\mathrm{th}$ row and $p-\mathrm{th}$ column of $(A - uv^T)^{-1}$.

The following example illustrates this procedure.

Let A and A^{-1} be

$$A = \begin{pmatrix} 1 & 4 & 6 \\ 2 & -1 & 3 \\ 3 & 2 & 5 \end{pmatrix},\ A^{-1} = \frac{1}{27}\begin{pmatrix} -11 & -8 & 18 \\ -1 & -13 & 9 \\ 7 & 10 & -9 \end{pmatrix}.$$

Let $A_{\bar{2},\bar{3}} = \begin{pmatrix} 1 & 4 \\ 3 & 2 \end{pmatrix}$, then

$$u = A_3 - e_2 = (6, 3-1, 5)^T, \qquad v = (0, 0, 1)^T,$$

and

$$A - uv^T = \begin{pmatrix} 1 & 4 & 0 \\ 2 & -1 & 1 \\ 3 & 2 & 0 \end{pmatrix}.$$

Since $A - uv^T$ is invertible, by using the Sherman-Morrison formula we obtain

$$(A - uv^T)^{-1} = \frac{1}{27}\begin{pmatrix} -11 & -8 & 18 \\ -1 & -13 & 9 \\ 7 & 10 & -9 \end{pmatrix} + \frac{\left(\frac{1}{27}\begin{pmatrix} -11 & -8 & 18 \\ -1 & -13 & 9 \\ 7 & 10 & -9 \end{pmatrix}\begin{pmatrix} 6 \\ 2 \\ 5 \end{pmatrix}\right)\left((0,0,1)\frac{1}{27}\begin{pmatrix} -11 & -8 & 18 \\ -1 & -13 & 9 \\ 7 & 10 & -9 \end{pmatrix}\right)}{1 - (0,0,1)\frac{1}{27}\begin{pmatrix} -11 & -8 & 18 \\ -1 & -13 & 9 \\ 7 & 10 & -9 \end{pmatrix}\begin{pmatrix} 6 \\ 2 \\ 5 \end{pmatrix}}$$
$$= \frac{1}{10}\begin{pmatrix} -2 & 0 & 4 \\ 3 & 0 & -1 \\ 7 & 1 & -9 \end{pmatrix}.$$

By eliminating the $3\mathrm{rd}$ row and the $2\mathrm{nd}$ column, we obtain

$$(A - uv^T)^{-1}_{\bar{3};\bar{2}} = \frac{1}{10}\begin{pmatrix} -2 & 4 \\ 3 & -1 \end{pmatrix} = A_{\bar{2};\bar{3}}^{-1},$$

which is the inverse of the submatrix.

If the number of additions and subtractions (NAS) and the number of multiplications and divisions (NMD) are considered separately, the Sherman-Morrison formula provides a method for calculating the inverse of a submatrix of order $n-1$, with

$$NAS = 2n(2n-1);\ NMD = n(5n+1), \qquad (4)$$

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where n is the order of the original matrix. The result is obtained by doing a simple sum of each algebraic operation performed on the different steps of the algorithm.

In this paper, we show a simpler, more direct formula with

$$NAS = (n-1)(n-1); \quad NMD = 2(n-1)(n-1). \tag{5}$$

The paper is organized as follows. In the next section, we show a formula for calculating each element of the inverse of a non-singular submatrix of order $n-1$ in terms of the elements of the inverse of the original matrix. An example of the use of the formula is illustrated in Section 3. The formula is implemented computationally in Section 4 on MatLab and Fortran 90 for a Fourier matrix, comparing the formula's runtime with respect to the already implemented algorithms in each programming language that are based on LU decomposition. Then, in Section 5, a general formula for the inverse of any square submatrix of a given $n \times n$ matrix is obtained. Finally, in Section 6, the relationship between the inverses of block submatrices and their original matrix, which was used in [8, 22, 25], is derived.

2 Submatrices of Order $n-1$

In the sequel, we consider the vector space $F^{n\times n}$ of matrices over the real or complex field.

Let $A \in F^{n\times n}$, $A = (a_{ij}),\ i,j = 1,\dots,n$ be invertible, and let $A^{-1} = (b_{ij}),\ i,j = 1,\dots,n$ be its inverse. Then, we obtain

$$b_{ij} = (-1)^{i+j}\frac{\det A_{\bar{j};\bar{i}}}{\det A}. \tag{6}$$

Let $M = A_{\bar{p};\bar{q}}$ be a submatrix of A. For our purposes, we will use the following notation:

$$M = (a_{ij}),\ i = 1,\dots,p-1,p+1,\dots,n,\ j = 1,\dots,q-1,q+1,\dots,n,$$

or, in short,

$$M = (a_{ij}),\ i,j = 1{:}n, i \neq p, j \neq q.$$

Note that $A_{\bar{p};\bar{q}}$ is invertible $\Leftrightarrow$ $b_{qp} \neq 0$.

Next, we derive the formula for the calculation of the inverse of $M^{-1} = (m_{ij})$.

Theorem 2.1. *Let $A = (a_{ij})$ be a nonsingular matrix of order n, and let $A^{-1} = (b_{ij})$ be its inverse. If a_{pq} and b_{qp} are both not null for certain $p, q \in \{1,\dots,n\}$, then the submatrix $M = A_{\bar{p};\bar{q}}$ is invertible, and its inverse $M^{-1} = (m_{ij})$ is a matrix of order $(n-1)$ defined as*

$$m_{ij} = b_{ij} - \frac{b_{ip}b_{qj}}{b_{qp}}, i,j = 1{:}n, i \neq q, j \neq p. \tag{7}$$

Proof. Since A^{-1} is the inverse of A and, reciprocally, $A^{-1}A = AA^{-1} = I_n$, where I_n is the identity matrix of order n. Thus,

$$\forall i,j = 1{:}n, \sum_{k=1}^{n} b_{ik}a_{kj} = \delta_{ij},$$

$$\forall i,j = 1{:}n, \sum_{k=1}^{n} a_{ik}b_{kj} = \delta_{ij},$$

where δ_{ij} is the Kronecker's delta, being equal to 1 if $i = j$ and to 0 if $i \neq j$. These equations can be expressed as

$$\forall i,j = 1{:}n, \quad \sum_{k=1,k\neq p}^{n} b_{ik}a_{kj} = \delta_{ij} - b_{ip}a_{pj}, \tag{8}$$

$$\forall i,j = 1{:}n, \quad \sum_{k=1,k\neq q}^{n} a_{ik}b_{kj} = \delta_{ij} - a_{iq}b_{qj}. \tag{9}$$

We define $D = (d_{ij}) \in F^{(n-1)\times(n-1)}$ as the matrix

$$d_{ij} := \delta_{ij} - b_{ip}a_{pj}, i,j = 1{:}n;\ i \neq q, j \neq q,$$

where p and q indicate the number of the row and the column, respectively, which are eliminated from matrix A to obtain the submatrix $M = A_{\bar{p};\bar{q}}$.

Matrix D can be expressed as

$$D = I_{n-1} - uv^T, \tag{10}$$

where $u = \left(b_{1p},\dots,b_{(q-1)p},b_{(q+1)p}\dots,b_{np}\right)^T$ is the $p-th$ column of A^{-1} after eliminating its $q-\text{th}$ component. Analogously, vector $v =$

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$\left(a_{p1}, \dots, a_{p(q-1)}, a_{p(q+1)} \dots, a_{pn}\right)^T$ is the $p-\text{th}$ row of matrix A after eliminating its $q-\text{th}$ component.

The inverse of D in Eq. (10) can be calculated by using the Sherman-Morrison formula (1), which contains the scalar $1 - v^T u$, and by using Eq. (9) we can see that

$$1 - v^T u = 1 - \sum_{k=1,k\neq q}^{n} a_{pk} b_{kp} = a_{pq} b_{qp}.$$

Thus, if $a_{pq} b_{qp} \neq 0$ (i.e., both a_{pq} and b_{qp} are nonzero), D is invertible and, according to Eq. (1), we obtain

$$D^{-1} = [I_{n-1} - uv^T]^{-1} = I_{n-1} + \frac{uv^T}{1 - v^T u}$$
$$= I_{n-1} + \frac{uv^T}{a_{pq} b_{qp}}.$$

On the other hand, D can be expressed as a matrix form by using Eq. (8) such that

$$NM = D, \quad (11)$$

where N is the submatrix of A^{-1} defined as

$$N = A^{-1}_{\bar{q};\bar{p}} = (b_{ij}),$$
$$i,j = 1{:}n, \quad i \neq q, \quad j \neq p. \quad (12)$$

According to Eq. (11), $D^{-1}NM = I_{n-1}$. Then,

$$M^{-1} = D^{-1}N = N + \frac{uv^T N}{a_{pq} b_{qp}}.$$

Substituting u, v^T and using matrix N in Eq. (12), the elements m_{ij} of matrix M^{-1} are given by

$$m_{ij} = b_{ij} + \frac{b_{ip}}{a_{pq} b_{qp}} \sum_{k\neq q} a_{pk} b_{kj},$$
$$i,j = 1{:}n, i \neq q, j \neq p.$$

Finally, using Eq. (9) we obtain the formula

$$m_{ij} = b_{ij} - \frac{b_{ip} b_{qj}}{b_{qp}}, i,j = 1{:}n, i \neq q, j \neq p. \blacksquare$$

In this theorem, the condition $a_{pq} \neq 0$ is necessary due to the use of the Sherman-Morrison formula; however, this hypothesis is removed in the theorem below.

Theorem 2.2. *Let* A *be an invertible matrix of order* n*, and let* $A^{-1} = (b_{ij})$ *be its inverse. If* $b_{qp} \neq 0$ *for some* $q,p \in \{1,\dots,n\}$*, then* $M = A_{\bar{p};\bar{q}}$ *is invertible and its inverse* $M^{-1} = (m_{ij})$ *is given by Eq. (7).*

Proof. It is sufficient to prove that submatrices M and M^{-1} satisfy the relation $M^{-1}M = I_{n-1}$ (see [6]). Since $M = (a_{ij})$, $i,j = 1{:}n, i \neq p, j \neq q$ and $M^{-1} = (m_{ij})$, $i,j = 1{:}n, i \neq q, j \neq q$, the elements of their product $M^{-1}M = (c_{ij})$ are

$$c_{ij} = \sum_{k=1,k\neq p}^{n} m_{ik} a_{kj}, i,j = 1{:}n, i \neq q, j \neq q.$$

Substituting m_{ik} in Eq. (7),

$$c_{ij} = \sum_{k=1,k\neq p}^{n} \left(b_{ik} - \frac{b_{ip} b_{qk}}{b_{qp}}\right) a_{kj}$$
$$= \sum_{k=1,k\neq p}^{n} b_{ik} a_{kj} - \sum_{k=1,k\neq p}^{n} \frac{b_{ip} b_{qk}}{b_{qp}} a_{kj}$$
$$= \sum_{k=1,k\neq p}^{n} b_{ik} a_{kj} - \frac{b_{ip}}{b_{qp}} \sum_{k=1,k\neq p}^{n} b_{qk} a_{kj}.$$

by Eq. (8)

$$= \delta_{ij} - b_{ip} a_{pj} - \frac{b_{ip}}{b_{qp}} \left(\delta_{qj} - b_{qp} a_{pj}\right)$$
$$= \delta_{ij} - b_{ip} a_{pj} - \frac{b_{ip}}{b_{qp}} \delta_{qj} + b_{ip} a_{pj} = \delta_{ij}.$$

since $j \neq q$, we obtain $\delta_{qj} = 0$. ■

By doing a simple sum of the operations required to obtain the inverse of submatrix $M = A_{\bar{p};\bar{q}}$ in Eq. (7), NAS and NMD are confirmed to be as in Eq. (5).

3 Example

Consider the DFT $\mathcal{F}$ of the sequence of n complex numbers $x_0, \dots, x_{n-1}$ into the n complex numbers $y_0, \dots, y_{n-1}$ according to the formula:

$$y_k = \sum_{m=0}^{n-1} x_m \, e^{-\frac{2\pi i}{n}km}, k = 0{:}\,(n-1).$$

This linear transformation can be expressed in terms of the $n \times n$ Vandermonde matrix F as

$$y = \mathcal{F}\{x\} = Fx,$$

where $y = (y_0, \dots, y_{n-1})^T$, $x = (x_0, \dots, x_{n-1})^T \in \mathbb{C}^n$, and F is

$$F = \begin{pmatrix} \left(e^{-\frac{2\pi i}{n}}\right)^{0(0)} & \cdots & \left(e^{-\frac{2\pi i}{n}}\right)^{0(n-1)} \\ \vdots & \ddots & \vdots \\ \left(e^{-\frac{2\pi i}{n}}\right)^{(n-1)(0)} & \cdots & \left(e^{-\frac{2\pi i}{n}}\right)^{(n-1)(n-1)} \end{pmatrix}. \quad (13)$$

The inverse of matrix F corresponds to the Inverse Discrete Fourier Transform

$$x = \mathcal{F}^{-1}\{y\} = F^{-1}y,$$

where F^{-1} is given by $F^{-1} = \frac{1}{n}F^*$ (the asterisk denotes complex conjugate):

$$F^{-1} = \frac{1}{n}\begin{pmatrix} \left(e^{\frac{2\pi i}{n}}\right)^{0(0)} & \cdots & \left(e^{\frac{2\pi i}{n}}\right)^{0(n-1)} \\ \vdots & \ddots & \vdots \\ \left(e^{\frac{2\pi i}{n}}\right)^{(n-1)(0)} & \cdots & \left(e^{\frac{2\pi i}{n}}\right)^{(n-1)(n-1)} \end{pmatrix}.$$

Now, let us apply Theorem 2.2 to calculate the inverses of submatrices of order $n-1$ of the matrix F in Eq. (13). To achieve this purpose, it is convenient to express matrices F and F^{-1} in the form

$$F = (f_{kl}), \;\; f_{kl} = \left(e^{-\frac{2\pi i}{n}}\right)^{(k-1)(l-1)}, \quad k, l = 1{:}\,n \quad (14)$$

$$F^{-1} = (g_{kl}), \;\; g_{kl} = \frac{1}{n}\left(e^{\frac{2\pi i}{n}}\right)^{(k-1)(l-1)}, \;\; k, l = 1{:}\,n.$$

Note that $g_{qp} \neq 0$, for all $q, p \in \{1, \dots, n\}$, then any submatrix $M = F_{\bar{p};\bar{q}}$ of F is invertible by using Theorem 2.2, and its inverse $M^{-1} = (m_{kl})$ is given by (7) as

$$m_{kl} = \frac{1}{n}\left(e^{\frac{2\pi i}{n}}\right)^{-(l+k-1)}\left[\left(e^{\frac{2\pi i}{n}}\right)^{kl} - \left(e^{\frac{2\pi i}{n}}\right)^{kp+ql-pq}\right], k, l = 1{:}\,n, k \neq q, l \neq p. \quad (15)$$

It should be emphasized that Eq. (15) provides the inverse of any submatrix of order $n-1$ of matrix F in (13).

For the specific case $n = 4$, F has the form

$$F = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & (-i)^1 & (-i)^2 & (-i)^3 \\ 1 & (-i)^2 & (-i)^4 & (-i)^6 \\ 1 & (-i)^3 & (-i)^6 & (-i)^9 \end{pmatrix},$$

or equivalently

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{pmatrix}.$$

And its inverse is given by

$$F^{-1} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i^1 & i^2 & i^3 \\ 1 & i^2 & i^4 & i^6 \\ 1 & i^3 & i^6 & i^9 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}.$$

$$M = F_{\bar{4};\bar{2}} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & i \\ 1 & 1 & -1 \end{pmatrix}.$$

i. If $M = F_{\bar{4};\bar{2}}$, then by using formula (15), we directly obtain

$$M^{-1} = \begin{pmatrix} \frac{1}{4}i^{-1}(i - i^{-2}) & \frac{1}{4}i^{-2}(i^2 - i^0) & \frac{1}{4}i^{-3}(i^3 - i^2) \\ \frac{1}{4}i^{-3}(i^3 - i^6) & \frac{1}{4}i^{-4}(i^6 - i^8) & \frac{1}{4}i^{-5}(i^9 - i^{10}) \\ \frac{1}{4}i^{-4}(i^4 - i^{10}) & \frac{1}{4}i^{-5}(i^8 - i^{12}) & \frac{1}{4}i^{-6}(i^{12} - i^{14}) \end{pmatrix}.$$

$$M = F_{\bar{4};\bar{4}} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -i & -1 \\ 1 & -1 & 1 \end{pmatrix}$$

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$$= \begin{pmatrix} \frac{1}{4}-\frac{1}{4}i & \frac{1}{2} & \frac{1}{4}+\frac{1}{4}i \\ \frac{1}{4}+\frac{1}{4}i & -\frac{1}{2} & \frac{1}{4}-\frac{1}{4}i \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix}.$$

ii. If $M = F_{\bar{4};\bar{4}}$ is a principal submatrix then we obtain

$$M^{-1} = \begin{pmatrix} \frac{1}{4}-\frac{\frac{1}{4}\left(\frac{1}{4}\right)}{\frac{i}{4}} & \frac{1}{4}-\frac{\frac{1}{4}\left(\frac{-i}{4}\right)}{\frac{i}{4}} & \frac{1}{4}-\frac{\frac{1}{4}\left(\frac{-1}{4}\right)}{\frac{i}{4}} \\ \frac{1}{4}-\frac{\frac{-i}{4}\left(\frac{1}{4}\right)}{\frac{i}{4}} & \frac{i}{4}-\frac{\frac{-i}{4}\left(\frac{-i}{4}\right)}{\frac{i}{4}} & -\frac{1}{4}-\frac{\frac{-i}{4}\left(\frac{-1}{4}\right)}{\frac{i}{4}} \\ \frac{1}{4}-\frac{\frac{-1}{4}\left(\frac{1}{4}\right)}{\frac{i}{4}} & -\frac{1}{4}-\frac{\frac{-1}{4}\left(\frac{-i}{4}\right)}{\frac{i}{4}} & \frac{1}{4}-\frac{\frac{-1}{4}\left(\frac{-1}{4}\right)}{\frac{i}{4}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{4}+\frac{1}{4}i & \frac{1}{2} & \frac{1}{4}-\frac{1}{4}i \\ \frac{1}{2} & 0 & -\frac{1}{2} \\ \frac{1}{4}-\frac{1}{4}i & -\frac{1}{2} & \frac{1}{4}+\frac{1}{4}i \end{pmatrix}.$$

4 Computational Implementation

First, we calculate the number of operations of the Sherman-Morrison method, formula in Eq. (7), and the LU algorithm. By using equations (4) and (5), the total number of operations to compute the matrix inverse with the Sherman-Morrison formula in Eq. (1) is $2n(2n-1)+n(5n+1)=9n^2-n=O(n^2)$; with the formula in Eq. (7), $3(n-1)^2=O(n^2)$; and with LU Decomposition, $O(n^3)$ operations are required [2]. In the specific case of Vandermonde matrices, we need $6n^2$ flops.

Although the number of operations with the Sherman-Morrison formula and the formula in Eq. (7) are of the same order, the slopes of the polynomial functions given by the number of operations of each method are 18 and 6, respectively, so we argue that the algorithm provided in this paper is more efficient. With the Vandermonde matrices, the slope of the function given by the number of operations is 12.

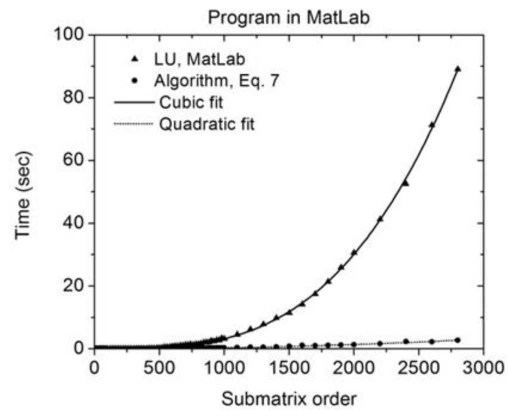

Fig. 1. Implementation of Equation (7) in comparison to the LU algorithm on MatLab

In the remaining part of this section, we compare the results of the implementation of formula (7) with LU MatLab algorithm on v.R2008a and Fortran 90 for the specific case of Vandermonde matrices of DFT (see Section 3). The algorithms were executed on a notebook with 2.27 GHz Intel Core i3 processor and a 4 GB RAM memory.

To implement the algorithm, row 4 and column 2 were eliminated in order to obtain the submatrix of order $n-1$.

Figure 1 shows the results of comparing the matrix size with runtime on MatLab. For matrices of order 600 approximately, the algorithm performance in Equation (7) is similar to the performance of MatLab's LU algorithm. However, for higher orders, the traditional algorithm requires higher runtimes, whereas formula (7) maintains small values for matrices of order 3×10^3 approximately.

In this case, the runtime is about 3 seconds in comparison to 90 seconds of the LU algorithm.

In Figure 2, the implementation results in Fortran 90 are presented. Note that the same pattern with the runtime variant increases significantly. Therefore, for a matrix of order 3×10^3 approximately, the LU algorithm runtime is about 1300 seconds.

Finally, in Figure 3, the performance of Equation (7) in both computational programs is exposed. Note that there is no significant difference on runtime performance, obtaining values of the same order of magnitude. For

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matrices of order 3×10^3 approximately, the runtime does not exceed three seconds. This is an indicator that algorithm performance does not depend on software.

5 Submatrices of Order $n-k$

5.1. Iterative Procedure

The derived relation (7) between the inverse of a submatrix $A_{\bar{p};\bar{q}}$ of order $n-1$ with the inverse $A^{-1} = (b_{ij})$ of the original matrix A can be iteratively applied to calculate the inverse of a submatrix of order $(n-k),\ 1 \le k < n$.

Let $M_k = A_{\overline{p_1},\cdots,\overline{p_k};\overline{q_1},\cdots,\overline{q_k}}$ be a submatrix of order $(n-k)$ obtained from a matrix A of order n by eliminating its $p_1-,\ldots,p_k-\text{th}$ rows and its $q_1-,\ldots,q_k-\text{th}$ columns. Then, the inverse $M_k^{-1} = \left(m_{ij}^{(k)}\right)$ of the submatrix M_k can be obtained by applying the iterative procedure:

$$\begin{aligned} m_{ij}^{(1)} &= b_{ij} - \frac{b_{ip_1} b_{q_1 j}}{b_{q_1 p_1}}, \\ i,j &= 1{:}n, i \ne q_1, j \ne p_1, \\ m_{ij}^{(2)} &= m_{ij}^{(1)} - \frac{m_{ip_2}^{(1)} m_{q_2 j}^{(1)}}{m_{q_2 p_2}^{(1)}}, \\ i,j &= 1{:}n, i \ne q_1, q_2,\ \ j \ne p_1, p_2, \\ m_{ij}^{(k)} &= m_{ij}^{(k-1)} - \frac{m_{ip_k}^{(k-1)} m_{q_k j}^{(k-1)}}{m_{q_k p_k}^{(k-1)}}, \\ i,j &= 1{:}n, i \ne q_1, \ldots, q_k\ \ j \ne p_1,, \ldots, p_k. \end{aligned} \tag{16}$$

This algorithm is applicable by using Theorem 2.2 if

$$b_{q_1 p_1} \ne 0, m_{q_2 p_2}^{(1)} \ne 0, \cdots, m_{q_k p_k}^{(k-1)} \ne 0, \tag{17}$$

i.e., all submatrices $M_l, (l = 1{:}k)$ are invertible.

5.2 General Formula

Let us apply the iterative procedure described above to obtain explicit expressions for the elements $m_{ij}^{(l)}$ of the inverses of square submatrices in terms of determinants containing the elements b_{ij} of A^{-1}.

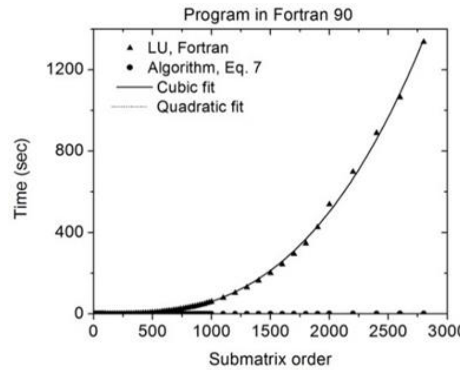

Fig. 2. Implementation of Eq. (7) in comparison to the LU algorithm on Fortran 90

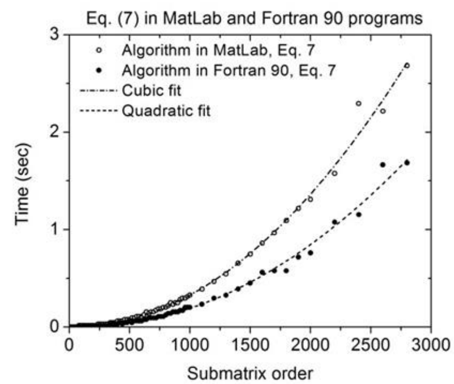

Fig. 3. Computational comparison between MatLab and Fortran 90 programs

Case M_1. We can express formula (7) for $m_{ij}^{(1)}$ of matrix M_1^{-1} in (16) as follows:

$$m_{ij}^{(1)} = \frac{b_{q_1 p_1} b_{ij} - b_{ip_1} b_{q_1 j}}{b_{q_1 p_1}} = \frac{\begin{vmatrix} b_{q_1 p_1} & b_{q_1 j} \\ b_{ip_1} & b_{ij} \end{vmatrix}}{b_{q_1 p_1}}. \tag{18}$$

In particular, $m_{q_2 p_2}^{(1)}$ is given by

$$m_{q_2 p_2}^{(1)} = \frac{\begin{vmatrix} b_{q_1 p_1} & b_{q_1 p_2} \\ b_{q_2 p_1} & b_{q_2 p_2} \end{vmatrix}}{b_{q_1 p_1}}. \tag{19}$$

Case M_2. Consider the invertible submatrix $M_1 = A_{\overline{p_1};\overline{q_1}}$ (i.e., $b_{q_1 p_1} \ne 0$), and let $M_1^{-1} = \left(m_{ij}^{(1)}\right)$

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be its inverse. Let $p_2, q_2 \in \{1, \dots, n\}$ such that $p_1 \neq p_2, q_1 \neq q_2$. If the element $m^{(1)}_{q_2 p_2}$ (17) of the matrix M_1^{-1} is not null ($m^{(1)}_{q_2 p_2} \neq 0$), then the submatrix $M_2 = A_{\overline{p_1}, \overline{p_2}; \overline{q_1}, \overline{q_2}}$ of order $(n-2)$, obtained from $M_1 = A_{\overline{p_1}; \overline{q_1}}$ by eliminating its p_2-th row and q_2-th column, is invertible. By (16) and (18), the elements $m^{(2)}_{ij}$ of matrix M_2^{-1} can be expressed as

$$\frac{\begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{vmatrix} \begin{vmatrix} b_{q_1p_1} & b_{q_1j} \\ b_{ip_1} & b_{ij} \end{vmatrix} - \begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{ip_1} & b_{ip_2} \end{vmatrix} \begin{vmatrix} b_{q_1p_1} & b_{q_1j} \\ b_{q_2p_1} & b_{q_2j} \end{vmatrix}}{b_{q_1p_1} \begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{vmatrix}}.$$

After simplifying, we obtain

$$m^{(2)}_{ij} = \frac{b_{q_1p_1}\left(b_{q_2p_2} b_{ij} - b_{ip_2} b_{q_2j}\right)}{\begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{vmatrix}} - \frac{b_{q_1p_2}\left(b_{ij} b_{q_2p_1} - b_{ip_1} b_{q_2j}\right)}{\begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{vmatrix}} + \frac{b_{q_1j}\left(b_{q_2p_1} b_{ip_2} - b_{ip_1} b_{q_2p_2}\right)}{\begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{vmatrix}}.$$

Thus,

$$m^{(2)}_{ij} = \frac{\begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} & b_{q_1j} \\ b_{q_2p_1} & b_{q_2p_2} & b_{q_2j} \\ b_{ip_1} & b_{ip_2} & b_{ij} \end{vmatrix}}{\begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{vmatrix}},$$
$$i, j = 1{:}n, i \neq q_1, q_2, \ \ j \neq p_1, p_2.$$

In this case, therefore, we have the following theorem.

Theorem 5.1. *Let A be a nonsingular matrix of order $n \geq 3$, and let $A^{-1} = (b_{ij})$ be its inverse. If the submatrix of order 2*

$$\begin{pmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{pmatrix} \tag{20}$$

of A^{-1} has non-null leading principal minors, for certain $p_1, p_2, q_1, q_2 \in \{1, 2, \dots, n\}$ with $p_1 \neq p_2$, $q_1 \neq q_2$, then $M_2 = A_{\overline{p_1}, \overline{p_2}; \overline{q_1}, \overline{q_2}}$ is invertible and its inverse $M_2^{-1} = \left(m^{(2)}_{ij}\right)$ is given by

$$\frac{\begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} & b_{q_1j} \\ b_{q_2p_1} & b_{q_2p_2} & b_{q_jj} \\ b_{ip_1} & b_{ip_2} & b_{ij} \end{vmatrix}}{\begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{vmatrix}}, \tag{21}$$
$$i, j = 1{:}n, i \neq q_1, q_2, \ \ j \neq p_1, p_2 m^{(2)}_{ij}.$$

Proof. The leading principal minors of submatrix (20) are:

$$b_{q_1p_1}, \begin{vmatrix} b_{q_1p_1} & b_{q_1p_2} \\ b_{q_2p_1} & b_{q_2p_2} \end{vmatrix}.$$

If these minors are different from zero, then $m^{(1)}_{q_2p_2}$ in (19) is not null. Subsequently, if conditions in (17) ($b_{q_1p_1} \neq 0$, $m^{(1)}_{q_2p_2} \neq 0$) are fully satisfied, then M_2 is invertible. The elements of M_2^{-1} can be calculated by using formulas in (16), which can be expressed again in the form of (21).■

Case M_k. The above results obtained for cases M_1 and M_2 allow us to infer a general formula for M_k, with $1 \leq k < n$.

Theorem 5.2. *Let A be a nonsingular matrix of order n, and let $A^{-1} = (b_{ij})$ be its inverse. Let $k \in N$ such that $k < n$. If the submatrix of order $k \times k$*

$$\begin{pmatrix} b_{q_1p_1} & b_{q_1p_2} & \cdots & b_{q_1p_k} \\ b_{q_2p_1} & b_{q_2p_2} & \cdots & b_{q_2p_k} \\ \vdots & \vdots & \ddots & \vdots \\ b_{q_kp_1} & b_{q_kp_2} & \cdots & b_{q_kp_k} \end{pmatrix} \tag{22}$$

of A^{-1} has non-null leading principal minors for certain $p_1, \dots, p_k, q_1, \dots, q_k \in \{1, \dots, n\}$ satisfying $p_{j_1} \neq p_{j_2}$ for $j_1 \neq j_2$ and $q_{i_1} \neq q_{i_2}$ for $i_1 \neq i_2$, then the submatrix $M_k = A_{\overline{p_1}, \cdots, \overline{p_k}; \overline{q_1}, \cdots, \overline{q_k}}$ of A is invertible and its inverse $M_k^{-1} = \left(m^{(k)}_{ij}\right)$ is a matrix of order $(n-k)$ with elements defined by

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$$m_{ij}^{(k)} = \frac{\begin{vmatrix} b_{q_1p_1} & \cdots & b_{q_1p_k} & b_{q_1j} \\ \vdots & \ddots & \vdots & \vdots \\ b_{q_kp_1} & \cdots & b_{q_kp_k} & b_{q_kj} \\ b_{ip_1} & \cdots & b_{ip_k} & b_{ij} \end{vmatrix}}{\begin{vmatrix} b_{q_1p_1} & \cdots & b_{q_1p_k} \\ \vdots & \ddots & \vdots \\ b_{q_kp_1} & \cdots & b_{q_kp_k} \end{vmatrix}}, \qquad (23)$$

$$i,j = 1,\ldots,n, i \neq q_1,\ldots,q_k, j \neq p_1,\ldots,p_k.$$

Proof. Let us demonstrate the theorem by mathematical induction.

Step 1. Let us verify that the proposition of the theorem is true for case M_1. If the 1×1 submatrix

$$\left(b_{q_1p_1}\right)$$

of A^{-1} has non-null leading principal minors, i.e., $b_{q_1p_1} \neq 0$, then the submatrix $M_1 = A_{\overline{p_1};\overline{q_1}}$ is invertible and its inverse $M_1^{-1} = \left(m_{ij}^{(1)}\right)$ is given by formula (7) from Theorem 2.2. The general expression (23) is another form of Eq. (7) as shown in Eq. (18).

Step 2. Let us suppose that the proposition is true for case M_{k-1}. Thus, if the submatrix of A^{-1} of order $k-1$

$$\begin{pmatrix} b_{q_1p_1} & \cdots & b_{q_1p_k} \\ \vdots & \ddots & \vdots \\ b_{q_{k-1}p_1} & \cdots & b_{q_{k-1}p_{k-1}} \end{pmatrix}$$

has non-null leading principal minors, the submatrix $M_{k-1} = A_{\overline{p_1},\cdots,\overline{p_{k-1}};\overline{q_1},,\cdots,\overline{q_{k-1}}}$ of A is invertible and its inverse $M_{k-1}^{-1} = \left(m_{ij}^{(k-1)}\right)$ is the matrix of order $(n-k+1)$ given by

$$m_{ij}^{(k-1)} = \frac{\begin{vmatrix} b_{q_1p_1} & \cdots & b_{q_1p_{k-1}} & b_{q_1j} \\ \vdots & \ddots & \vdots & \vdots \\ b_{q_{k-1}p_1} & \cdots & b_{q_{k-1}p_{k-1}} & b_{q_{k-1}j} \\ b_{ip_1} & \cdots & b_{ip_{k-1}} & b_{ij} \end{vmatrix}}{\begin{vmatrix} b_{q_1p_1} & \cdots & b_{q_1p_{k-1}} \\ \vdots & \ddots & \vdots \\ b_{q_{k-1}p_1} & \cdots & b_{q_{k-1}p_{k-1}} \end{vmatrix}}, \qquad (24)$$

$$i,j = 1{:}n, i \neq q_1,\ldots,q_{k-1},\ j \neq p_1,\ldots,p_{k-1}.$$

If the conditions in (17) are satisfied, the elements $m_{ij}^{(k)}$ of matrix M_k^{-1} are expressed in terms of the elements $m_{ij}^{(k-1)}$ of M_{k-1}^{-1} according to Eq. (16). Such conditions demand that leading principal minors of matrix (22) be non-null. In fact, note that the elements $b_{q_1p_1}, m_{q_2p_2}^{(1)}, \cdots, m_{q_kp_k}^{(k-1)}$, appearing in the denominators of Eq. (16), turn out to be proportional to those minors, see Eq. (24). In the sequel, we denote the elements $m_{ij}^{(k)}$ (16) as

$$\begin{aligned} m_{ij}^{(k)} &= \frac{m_{q_kp_k}^{(k-1)} m_{ij}^{(k-1)} - m_{ip_k}^{(k-1)} m_{q_kj}^{(k-1)}}{m_{q_kp_k}^{(k-1)}} \\ &= \frac{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}\begin{vmatrix} A & U_2 \\ V_2 & D_2 \end{vmatrix} - \begin{vmatrix} A & U_1 \\ V_2 & D_3 \end{vmatrix}\begin{vmatrix} A & U_2 \\ V_1 & D_4 \end{vmatrix}}{|A|\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}}, \end{aligned} \qquad (25)$$

where we have used the following notation:

$$A = \begin{pmatrix} b_{q_1p_1} & \cdots & b_{q_1p_{k-1}} \\ \vdots & \ddots & \vdots \\ b_{q_{k-1}p_1} & \cdots & b_{q_{k-1}p_{k-1}} \end{pmatrix},$$

$$U_1 = \left(b_{q_1p_k} \quad b_{q_2p_k} \cdots \quad b_{q_{k-1}p_k}\right)^T,$$

$$U_2 = \left(b_{q_1j} \quad b_{q_2j} \cdots \quad b_{q_{k-1}j}\right)^T,$$

$$V_1 = \left(b_{q_kp_1} \quad b_{q_kp_2} \cdots \quad b_{q_kp_{k-1}}\right),$$

$$V_2 = \left(b_{ip_1} \quad b_{ip_2} \cdots \quad b_{ip_{k-1}}\right),$$

$$D_1 = b_{q_kp_k}, D_2 = b_{ij}, \qquad D_3 = b_{ip_k}, D_4 = b_{q_kj}.$$

Using Eq. (2) for the determinant of a block-partitioned matrix (3), we directly obtain

$$\begin{aligned} m_{ij}^{(k)} &= \frac{|A|(D_1 - V_1A^{-1}U_1)(D_2 - V_2A^{-1}U_2)}{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}} \\ &- \frac{|A|(D_3 - V_2A^{-1}U_1)(D_4 - V_1A^{-1}U_2)}{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}}. \end{aligned} \qquad (26)$$

This result agrees with formula (23). In fact, by expressing (23) as

$$m_{ij}^{(k)} = \frac{\begin{vmatrix} A & U_1 & U_2 \\ V_1 & D_1 & D_4 \\ V_2 & D_3 & D_2 \end{vmatrix}}{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}}$$

and using Eq. (2) for the determinant of a block-partitioned matrix (3), we directly obtain

$$m_{ij}^{(k)} = \frac{|A|(D_1 - V_1A^{-1}U_1)(D_2 - V_2A^{-1}U_2)}{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}} - \frac{|A|(D_3 - V_2A^{-1}U_1)(D_4 - V_1A^{-1}U_2)}{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}}. \quad (26)$$

This result agrees with formula (23). In fact, by expressing (23) as

$$m_{ij}^{(k)} = \frac{\begin{vmatrix} A & U_1 & U_2 \\ V_1 & D_1 & D_4 \\ V_2 & D_3 & D_2 \end{vmatrix}}{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}}$$

and using Eq. (5), we obtain

$$m_{ij}^{(k)} = \frac{\det A \det\left[\begin{pmatrix} D_1 & D_4 \\ D_3 & D_2 \end{pmatrix} - \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} A^{-1}(U_1 \quad U_2)\right]}{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}}.$$

Subsequently, this formula is reduced to the expression

$$m_{ij}^{(k)} = \frac{|A| \det\begin{bmatrix} D_1 - V_1A^{-1}U_1 & D_4 - V_1A^{-1}U_2 \\ D_3 - V_2A^{-1}U_1 & D_2 - V_2A^{-1}U_2 \end{bmatrix}}{\begin{vmatrix} A & U_1 \\ V_1 & D_1 \end{vmatrix}},$$

which evidently agrees with (26). It implies that this proposition is true for all k values.■

Note that in the specific case of $k = n-1$ in Theorem 5.2, the submatrix $M_{n-1} = A_{\overline{p_1},\dots,\overline{p_{n-1}};\overline{q_1},\dots,\overline{q_{n-1}}}$ of A is a 1×1 matrix and its inverse is $M_{n-1}^{-1} = \left(m_{ij}^{(n-1)}\right)$, where

$$m_{ij}^{(n-1)} = \frac{\begin{vmatrix} b_{q_1p_1} & \cdots & b_{q_1p_{n-1}} & b_{q_1j} \\ \vdots & \ddots & \vdots & \vdots \\ b_{q_{n-1}p_1} & \cdots & b_{q_{n-1}p_{n-1}} & b_{q_{n-1}j} \\ b_{ip_1} & \cdots & b_{ip_{n-1}} & b_{ij} \end{vmatrix}}{\begin{vmatrix} b_{q_1p_1} & \cdots & b_{q_1p_{n-1}} \\ \vdots & \ddots & \vdots \\ b_{q_{n-1}p_1} & \cdots & b_{q_{n-1}p_{n-1}} \end{vmatrix}}, \quad (27)$$

$$i,j = 1{:}n, i \neq q_1,\dots,q_{n-1}, \qquad j \neq p_1,\dots,p_{n-1}.$$

Then, indexes i and j, respectively, take the remaining value from the integers in $\{1,\dots,n\}$. Permutating the rows and columns of the determinant in the numerator of expression (27), we obtain

$$m_{ij}^{(n-1)} = \frac{(-1)^{i+j}|A^{-1}|}{\left|A_{\overline{j}\overline{i}}^{-1}\right|}.$$

By using (6) to calculate the elements of the matrix inverse of A^{-1} ($(A^{-1})^{-1} = A$), we obtain the expected result

$$m_{ij}^{(n-1)} = \frac{1}{a_{ij}}.$$

6 Block Submatrices

We generalize the relationship between the inverses of a matrix and their submatrices, which is derived in Section 2, to the case of block-partitioned matrices having square blocks of the same size.

Theorem 6.1. *Let* $\mathbf{A} = (A_{ij})$ *be a nonsingular block matrix of order* ns*, and let* $\mathbf{A}^{-1} = (B_{ij})$ *be its inverse, where* B_{ij} *is a* $s \times s$ *square block matrix,* $(1 \leq i;\ j \leq n)$. *If* B_{qp} *is invertible for certain* $q,p \in \{1,\dots,n\}$, *then the block-partitioned submatrix* $\mathbf{M} = \mathbf{A}_{\overline{p}\overline{q}}$ *obtained by eliminating the* $p-\mathrm{th}$ *block row and the* $q-\mathrm{th}$ *block column of* $\mathbf{A}$ *is invertible, and its inverse* $\mathbf{M}^{-1} = (M_{ij})$ *of order* $(n-1)s$ *is given by*

$$M_{ij} = B_{ij} - B_{ip}B_{qp}^{-1}B_{qj}, \quad i,j = 1{:}n, i \neq q, j \neq p. \quad (28)$$

Proof. The demonstration follows the same procedure as Theorem 2.2.

7 Conclusions

In summary, we have obtained a formula (Eq. (7)) that allows us to calculate the inverse of a submatrix of order $(n-1)$ in terms of the inverse A^{-1} of the original $n\times n$ matrix A. By applying such a formula iteratively, we have been able to derive an explicit relationship (23) between the inverse of an arbitrary square submatrix and its inverse A^{-1}.

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In addition, we have tested the computational efficiency of the formula's runtime when compared with the LU Decomposition for the case of Fourier matrices. We have also generalized formula (5) for the case of inverses of block-partitioned matrices with square blocks of the same size s, see Eq. (28). The relationship in Eq. (28) is particularly useful when the known inverse of the matrix is a very large order ($ns \gg 1$), and it is necessary to calculate the inverse of a submatrix of order $(n-1)s$.

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