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ON AN INVERSE FORMULA OF A TRIDIAGONAL MATRIX

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Abstract. This paper provides an inverse formula freed of determinant expressions for a general tridiagonal matrix. This is viewed as an alternative version of the Usmani formula, which easily tends to blow up computationally. We discuss a number of different viewpoints regarding the proposed and Usmani's formulas, such as the proof method and the meaning of included terms, although our formula itself may be obtained by a simple transformation of Usmani's. A study of the limit elements based on the inverse formula and a numerical experiment for comparison with the other inverse methods are provided. In addition, we briefly discuss the inverse formula in the case of zero minors, which is illustrated by a numerical example.

1. Inverse formula of a tridiagonal matrix

Consider the inverse $Z_n = (z_{ij})_{i,j=1}^n = Y_n^{-1}$ of a general $n \times n$ tridiagonal matrix,

$$Y_n = (y_{ij})_{i,j=1}^n = \begin{pmatrix} \alpha_1 & \gamma_1 & 0 & \cdots & 0 \\ \beta_2 & \alpha_2 & \gamma_2 & \ddots & \vdots \\ 0 & \beta_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \gamma_{n-1} \\ 0 & \cdots & 0 & \beta_n & \alpha_n \end{pmatrix}. \tag{1}$$

This subject has been studied by many authors [2, 6, 16, 17, 10, 11, 3, 1, 4, 5, 12, etc.]. Let us classify several expressions for Z_n into the three characteristics: (i) convenience or simplicity of a formula itself, (ii) numerical aspects that the algorithm is fast in computation or has less numerical errors and (iii) asymptotic aspects for studying the limit form. The Usmani formula [16, 17] provides an elegant solution for Z_n,

$$z_{ij} = \begin{cases} (-1)^{i+j}\gamma_i \cdots \gamma_{j-1}\theta_{i-1}\phi_{j+1}/\theta_n, & i < j \\ \theta_{i-1}\phi_{i+1}/\theta_n, & i = j \\ (-1)^{i+j}\beta_{j+1}\cdots\beta_i\theta_{j-1}\phi_{i+1}/\theta_n, & i > j \end{cases}, \tag{2}$$

where θ_i's are $\theta_i = \alpha_i\theta_{i-1} - \gamma_{i-1}\beta_i\theta_{i-2}$, $i = 2, \ldots, n$ with $\theta_1 = \alpha_1$ and $\theta_0 = 1$, while ϕ_i's are $\phi_i = \alpha_i\phi_{i+1} - \gamma_i\beta_{i+1}\phi_{i+2}$, $i = n-1, \ldots, 1$ with $\phi_n = \alpha_n$ and $\phi_{n+1} = 1$. Usmani's

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formula has the advantage of (i), and in addition realizes a stable numerical computation for many cases if n is not too large or the entries (α_i , etc.) seldom influence n.

However, (2) encounters problems as follows: for example, let $\alpha_i = 2n$ and $\beta_i = \gamma_{i-1} = n$ temporarily to consider the case of $\alpha_i = O(n)$ and $\beta_i = O(n)$ depending on n. Such a condition often occurs for the Fisher information matrix, which is well-known in statistics, in high-dimensional statistical model estimation [15]. If n becomes larger than 150, θ_n easily tends to `infinity` computationally in home programming software with the maximum length of about 300 in digits of the decimal numbers. Then, (2) and the other determinant-based formula [6, 10, e.g.] fail to obtain Z_n numerically, although $|z_{ij}|$ is not greater than $O(1)$, because of $\max_i z_{ii} = 1/4 + 1/2n$ by $\theta_k = \phi_{n-k+1} = (k+1)n^k$. The LU factorization [3, 1, e.g.] and cyclic reduction method [9], which are in general preferred than (2) for numerical computation, have the advantage of (ii) in this example.

Further, to discuss (iii), consider a derivation of $\lim_{n\to\infty} z_{ij}$ under some α_i, β_i and γ_i. Because θ_i solved using the recursive relation is expressed as a sum of product integrals [8], it will be generally difficult to formulate the limit form of θ_i, that is, to investigate the limit of z_{ij} using (2). Also, the explicit form obtained based on the LU factorization and cyclic reduction is usually complicated, which makes studying the limit of z_{ij} difficult.

To deal with these three aspects (i)-(iii), we consider an alternative expression of (2).

THEOREM 1. *For a tridiagonal matrix Y_n of (1), define sequences f_ℓ and g_ℓ by*

$$f_\ell = \frac{-\gamma_\ell}{f_{\ell-1}\beta_\ell + \alpha_\ell}, \quad \ell = 1,2,\ldots,n \ (\beta_1 = 0), \tag{3a}$$

$$g_\ell = \frac{-\beta_\ell}{g_{\ell+1}\gamma_\ell + \alpha_\ell}, \quad \ell = n,n-1,\ldots,1 \ (\gamma_n = 0) \tag{3b}$$

with $f_0 = 0$ and $g_{n+1} = 0$, and a product integral p_{ki} by

$$p_{ki} = \begin{cases} \prod_{\ell=k}^{i-1} f_\ell & \text{if } k < i, \\ 1 & \text{if } k = i, \\ \prod_{\ell=i+1}^{k} g_\ell & \text{if } k > i. \end{cases} \tag{4}$$

Then, the (i,j)-th element of $Z_n = Y_n^{-1}$ is

$$z_{ij} = v_{ij}/(v_{ii}v_{jj}),$$

where

$$v_{ij} = p_{ij}\left(\beta_i p_{i-1,i} + \alpha_i + \gamma_i p_{i+1,i}\right). \tag{5}$$

In advance, note that (5) means

$$v_{ij} = p_{ij}v_{ii} \ \text{ and } \ v_{ii} = \beta_i f_{i-1} + \alpha_i + \gamma_i g_{i+1}, \tag{5'}$$

because a special case of (4) is

$$p_{i-1,i} = f_{i-1}, \ p_{ii} = 1, \ p_{i+1,i} = g_{i+1}. \tag{4'}$$

Theorem 1 provides some different viewpoints to (2); for example, it is free of the determinant expressions which easily tend to blow up computationally, so that it leads to more stable computation (ii) than a direct use of (2), similar to the LU factorization and cyclic reduction method. This advantage also appears to work well in a theoretical regard, such as (iii). In addition, because (3a) and (3b) are expressed by nonlinear Volterra integral equations closely related to an extended Fibonacci sequence, it is often easy to find their solution expressions for specified α_i, β_i and γ_i. Given such solutions, we will be able to study the limit form of a linear combination of z_{ij}. In order to support and compare several findings from Theorem 1, in particular on (iii), we provide a further formula derived in the case of symmetric matrix below.

COROLLARY 1. *Assume that Y_n of (1) is a symmetric tridiagonal matrix given by $\gamma_i = \beta_{i+1}$, $i = 1, \ldots, n-1$. Then, there are μ_i and δ_i, $i = 1, \ldots, n$ which provide*

$$\alpha_i = \frac{\mu_i}{(q_{i-1} - q_i)^2} + \frac{\mu_{i+1}}{(q_i - q_{i+1})^2} + \frac{\delta_i}{q_i^2} \text{ and } \beta_{i+1} = -\frac{\mu_{i+1}}{(q_i - q_{i+1})^2}, \tag{6}$$

where $\mu_{n+1} = 0$ ($\mu_{n+1}/(q_n - q_{n+1})^2 = 0$),

$$q_i = \textstyle\prod_{\ell=1}^{i} (1 - \mu_\ell / r_\ell) \quad \text{and} \quad r_i = \sum_{\ell=i}^{n} (\mu_\ell + \delta_\ell), \ i = 1, \ldots, n.$$

Using the sequences $\{\mu_i\}_{i=1}^n$ and $\{\delta_i\}_{i=1}^n$, the (i, j)-th element of Z_n is expressed as

$$z_{ij} = q_i q_j \textstyle\sum_{\ell=1}^{\min(i,j)} \mu_\ell / \{r_\ell (r_\ell - \mu_\ell)\}.$$

Corollary 1 may not be derived so directly from Theorem 1, but is located as a special case of Theorem 1 (see [15, Lemma 5]). Corollary 1 may be more convenient for studying (iii) than Theorem 1, if Y_n is at least symmetric. Note, however, that the sequences $\{\mu_i\}_{i=1}^n$ and $\{\delta_i\}_{i=1}^n$ satisfying (6) are not unique with no restriction, because δ_i and μ_i, $i = n, \ldots, 1$ are obtained automatically from any non-zero value of q_n. For these backgrounds, in this paper, we focus on Theorem 1 and establish the knowledge obtained from Theorem 1. A further investigation on the relationship between Theorem 1 and Corollary 1 is placed in a future study which follows this work.

The formulas as Theorem 1 and Corollary 1 had not been studied. However, when this paper was under reviewing, [7, Algorithms 4.1 and 4.2] proposed algorithms eventually arranged to Theorem 1, and they showed that the algorithms have a relatively smaller number of computational steps. This study was performed and approached from a different viewpoint, completely independently of [7]. Also, the advantages of Theorem 1 are not necessarily investigated fully yet, so that it is worth investigating how this formula is characterized in terms of (ii)-(iii). In Section 2, a motivated example for Theorem 1 is shown. In Section 3, the proofs of Theorem 1 and Corollary 1 are provided. We find out the advantages of (iii) in addition to (ii) on Theorem 1. This example is discussed in Section 4. Section 5 is helpful for explaining how Theorem 1 is adaptable when Y_n has zero minors and, as this result, why the algorithm proposed in this paper can be applied numerically without requiring the symbolic computation such as Algorithm 2 of [7].

2. A motivated example and symmetric tridiagonal case

In this section, we will examine the origin of Theorem 1 in order to discuss an implication of f_ℓ and g_ℓ. For simplicity, the subject is restricted to the symmetric tridiagonal case. An alternative expression of Theorem 1 is also given.

Assume that Y_n is a negative definite symmetric tridiagonal matrix given by $\gamma_\ell = \beta_{\ell+1}$, $\ell = 1,\ldots,n$. We considered the derivatives of a function G such that

$$G(x_i) = \max_{x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_n} F(x) \;\text{ for } F(x) = \tfrac{1}{2}x^{\mathrm{T}}Y_n x - x^{\mathrm{T}}u,$$

where $x = (x_1,\ldots,x_n)^{\mathrm{T}}$ and $u = (u_1,\ldots,u_n)^{\mathrm{T}}$. Let $F_\ell(x) = \partial F(x)/\partial x_\ell$. Because the condition to obtain G from F is

$$F_\ell(x) = \beta_\ell x_{\ell-1} + \alpha_\ell x_\ell + \beta_{\ell+1}x_{\ell+1} - u_\ell = 0 \text{ for } \ell = 1,\ldots,i-1,i+1,\ldots,n,$$

the first derivative of G is

$$dG(x_i)/dx_i = \textstyle\sum_{j=1}^{n} \frac{\partial F(x)}{\partial x_j}\frac{dx_j}{dx_i} = F_i(x) = \beta_i x_{i-1} + \alpha_i x_i + \beta_{i+1}x_{i+1} - u_i,$$

so that the second derivative of G is expressed by

$$\frac{d^2G(x_i)}{dx_i^2} = \beta_i\frac{dx_{i-1}}{dx_i} + \alpha_i + \beta_{i+1}\frac{dx_{i+1}}{dx_i} \tag{7a}$$

$$\text{or} \quad = \sum_{j=1}^{n}\frac{dx_j}{dx_i}\left\{\beta_j\frac{dx_{j-1}}{dx_i} + \alpha_j\frac{dx_j}{dx_i} + \beta_{j+1}\frac{dx_{j+1}}{dx_i}\right\} \tag{7b}$$

with $dx_0/dx_i = dx_{n+1}/dx_i = 0$. Here, (7a) and (7b) are derived from the fact that

$$\frac{d^2G(x_i)}{dx_i^2} = \frac{d}{dx_i}\left\{\textstyle\sum_{j=1}^{n}\frac{\partial F(x)}{\partial x_j}\frac{dx_j}{dx_i}\right\} \text{ or } = \textstyle\sum_{j,l}\left\{\frac{\partial^2F(x)}{\partial x_j\partial x_l}\frac{dx_j}{dx_i}\frac{dx_l}{dx_i} + \frac{\partial F(x)}{\partial x_j}\frac{d^2x_j}{dx_i^2}\right\}.$$

Next, we consider the derivatives dx_j/dx_i. This is usually obtained by applying the implicit mapping theorem to the condition $F_j(x) = \partial F(x)/\partial x_j = 0$ for $j \neq i$. However, there is a recursive relation that does not depend on a matrix expression. For example, given $F_1(x) = 0$, i.e. $\alpha_1x_1 + \beta_2x_2 = 0$, x_1 is a function of x_2. Hence,

$$\frac{dx_1}{dx_2} = -\frac{dF_1/dx_2}{dF_1/dx_1} = \frac{-\beta_2}{\alpha_1} = f_1.$$

In addition, for $\ell \geqslant 2$, given $F_\ell(x) = \beta_\ell x_{\ell-1} + \alpha_\ell x_\ell + \beta_{\ell+1}x_{\ell+1} = 0$, since x_ℓ is a function of $(x_{\ell-1}, x_{\ell+1})$ under the relation $x_{\ell-1} = x_{\ell-1}(x_\ell)$ already obtained by $F_{\ell-1}(x) = 0$, we have

$$\frac{dx_\ell}{dx_{\ell+1}} = -\frac{dF_\ell/dx_{\ell+1}}{dF_\ell/dx_\ell} = \frac{-dF_\ell/dx_{\ell+1}}{\frac{\partial F_\ell}{\partial x_\ell} + \frac{\partial F_\ell}{\partial x_{\ell-1}}\frac{dx_{\ell-1}}{dx_\ell}} = \frac{-\beta_{\ell+1}}{\alpha_\ell + \beta_\ell f_{\ell-1}} = f_\ell. \tag{8}$$

Inversely, g_n means dx_n/dx_{n-1} computed by $F_n(x) = 0$. Hence, by starting from $g_{n+1} = 0$, we recursively obtain

$$\frac{dx_\ell}{dx_{\ell-1}} = -\frac{dF_\ell/dx_{\ell-1}}{dF_\ell/dx_\ell} = \frac{-dF_\ell/dx_{\ell-1}}{\frac{\partial F_\ell}{\partial x_\ell} + \frac{\partial F_\ell}{\partial x_{\ell+1}}\frac{dx_{\ell+1}}{dx_\ell}} = \frac{-\beta_\ell}{\alpha_\ell + \beta_{\ell+1}g_{\ell+1}} = g_\ell. \tag{9}$$

Therefore, by the chain rule of differentiations, dx_j/dx_i is computed as

$$\frac{dx_j}{dx_i} = \begin{cases} \frac{dx_j}{dx_{j+1}} \frac{dx_{j+1}}{dx_{j+2}} \cdots \frac{dx_{i-1}}{dx_i} & \text{if } j \leqslant i-1 \\ \frac{dx_j}{dx_{j-1}} \frac{dx_{j-1}}{dx_{j-2}} \cdots \frac{dx_{i+1}}{dx_i} & \text{if } j \geqslant i+1 \end{cases}.$$

From (8) and (9), it is found that p_{ji} defined by (4) means dx_j/dx_i. This makes us understand that v_{ij} is obtained by $p_{ij}v_{ii} = (dx_i/dx_j)(dF_i(x)/dx_i) = dF_i(x)/dx_j$ because $F_i(x)$ is equal to $dG(x_i)/dx_i$ and then we have $v_{ii} = dF_i(x)/dx_i$ from (7a).

Finally, we consider the meaning of $1/v_{ii}$. Note that the Jacobian matrix of functions $(F_1(x),\ldots,F_n(x))$ is Y_n. If $\det(Y_n) \neq 0$, we have the inverse functions denoted by $x_1(F_1,\ldots,F_n),\cdots,x_n(F_1,\ldots,F_n)$. Then, by the derivative formula of the inverse function of several variables,

$$\text{the } (i,i)\text{-th element } z_{ii} \text{ of } Z_n = Y_n^{-1} \text{ means } \frac{\partial x_i(F_1,\ldots,F_n)}{\partial F_i}. \tag{10}$$

On the other hand, because of $v_{ii} = dF_i(x)/dx_i$, by the derivative formula of the inverse function of single variable, we have

$$\frac{dx_i}{dF_i(x)} = \frac{1}{dF_i(x)/dx_i} = \frac{1}{v_{ii}},$$

which provides the same result as (10).

A shortcoming of the form $z_{ij} = p_{ij}/v_{jj}$ obtained from Theorem 1 is that it is not immediately clear how to achieve a symmetry between z_{ij} and z_{ji}, which should be obtained in the case of a symmetric tridiagonal matrix. Lemma 1 below provides a transformation of v_{ij} to see such a symmetry easily. In addition, the proof of Lemma 1 shows that (7a) is equivalent to (7b) even in a general symmetric tridiagonal matrix without having to be negative or positive definite. The expression of v_{ij} in Lemma 1 was originally found by the covariance structure of a superposition of forward and backward Gaussian martingale processes [14].

LEMMA 1. *Assume that Y_n is symmetric, i.e. $\gamma_\ell = \beta_{\ell+1}$, $\ell = 1,\ldots,n-1$. Then, v_{ij} defined by (4) is expressed as*

$$v_{ij} = -\textstyle\sum_{k=2}^n \beta_k(p_{ki} - p_{k-1,i})(p_{kj} - p_{k-1,j}) + \sum_{k=1}^n (\alpha_k + \beta_k + \beta_{k+1}) p_{ki} p_{kj}$$

with $\beta_1 = 0$ and $\beta_{n+1} = 0$.

Proof of Lemma 1. The expression of v_{ij} in Lemma 1 is provided by a simple transformation of (7b) as follows:

$$\begin{aligned} v_{ij} &= -\textstyle\sum_{k=2}^n \beta_k\{p_{ki}p_{kj} - p_{ki}p_{k-1,j} - p_{k-1,i}p_{k,j} + p_{k-1,i}p_{k-1,j}\} \\ &\qquad + \textstyle\sum_{k=1}^n (\alpha_k + \beta_k + \beta_{k+1}) p_{ki} p_{kj} \\ &= \textstyle\sum_{k=1}^n \{\beta_k p_{ki} p_{k-1,j} + \beta_{k+1} p_{ki} p_{k+1,j} + \alpha_k p_{ki} p_{kj}\}, \end{aligned}$$

which corresponds to (7b). Next, we show that this reduces to (7a), i.e., it is equivalent to the definition of (4). Note the relation

$$\beta_k p_{k-1,j} + \alpha_k p_{kj} = -\beta_{k+1} p_{k+1,j} \text{ if } k \neq j,$$

as provided further below in (13a) and (13b). Applying this relation to v_{ij} decomposed into

$$\begin{aligned} v_{ij} = & \textstyle\sum_{k=1}^{j-1} \left\{\beta_k p_{k-1,j} + \alpha_k p_{kj}\right\} p_{ki} + \left(\beta_j p_{j-1,j} + \alpha_j p_{jj}\right) p_{ji} \\ & + \textstyle\sum_{k=j+1}^{n} \left\{\beta_k p_{k-1,j} + \alpha_k p_{kj}\right\} p_{ki} + \sum_{k=1}^{n} \beta_{k+1} p_{ki} p_{k+1,j}, \end{aligned}$$

we obtain the form of (4) as

$$\begin{aligned} v_{ij} &= -\sum_{k=1}^{j-1} \beta_{k+1} p_{k+1,j} p_{ki} + \left(\beta_j p_{j-1,j} + \alpha_j\right) p_{ji} - \sum_{k=j+1}^{n} \beta_{k+1} p_{k+1,j} p_{ki} + \sum_{k=1}^{n} \beta_{k+1} p_{ki} p_{k+1,j} \\ &= \left(\beta_j p_{j-1,j} + \alpha_j p_{jj} + \beta_{j+1} p_{j+1,j}\right) p_{ji}. \quad \square \end{aligned}$$

3. Theoretical justification of the main result

This section provides a proof of Theorem 1 and the related results.

Proof of Theorem 1. Letting $(s_{ij})_{i,j=1}^{n} = Y_n Z_n$, we will then show that

$$s_{ij} = \beta_i z_{i-1,j} + \alpha_i z_{ij} + \gamma_i z_{i+1,j} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}.$$

By the definition $z_{ij} = v_{ij}/(v_{ii}v_{jj})$, the (i,j)-th element of $Y_n Z_n$ is written as

$$s_{ij} = \frac{s_{ij}^{(1)}}{s_{ij}^{(2)}} = \frac{\beta_i v_{i-1,j} v_{ii} v_{i+1,i+1} + \alpha_i v_{ij} v_{i-1,i-1} v_{i+1,i+1} + \gamma_i v_{i+1,j} v_{i-1,i-1} v_{ii}}{v_{i-1,i-1} v_{ii} v_{i+1,i+1} v_{jj}}.$$

We discuss shrinkage of the numerator $s_{ij}^{(1)}$ below.

Applying (5'), i.e. $v_{kj} = p_{kj} v_{kk}$ for $k = i-1, i, i+1$ to $s_{ij}^{(1)}$, we have

$$s_{ij}^{(1)} = (\beta_i p_{i-1,j} + \alpha_i p_{ij} + \gamma_i p_{i+1,j}) v_{i-1,i-1} v_{ii} v_{i+1,i+1}. \tag{11}$$

Consider the case of $i = j$ in (11). Then, using (5), we can show that

$$s_{ii}^{(1)} = (\beta_i p_{i-1,i} + \alpha_i + \gamma_i p_{i+1,i}) v_{i-1,i-1} v_{ii} v_{i+1,i+1} = v_{i-1,i-1} v_{ii}^2 v_{i+1,i+1}.$$

This leads to $s_{ii} = 1$. Next, consider the case of $i \neq j$ in (11). Using (4), we find that

$$\beta_i p_{i-1,j} + \alpha_i p_{ij} + \gamma_i p_{i+1,j} = \begin{cases} (\beta_i f_{i-1} f_i + \alpha_i f_i + \gamma_i)\, p_{i+1,j} & \text{if } i+1 \leqslant j \\ (\beta_i + \alpha_i g_i + \gamma_i g_i g_{i+1})\, p_{i-1,j} & \text{if } j \leqslant i-1 \end{cases}. \tag{12}$$

Further, note that equations (3a) and (3b) defining f_ℓ and g_ℓ are translated to

$$\beta_\ell f_\ell f_{\ell-1} + \alpha_\ell f_\ell + \gamma_\ell = 0, \quad \ell = 1,2,\dots,n, \tag{13a}$$

$$\gamma_\ell g_\ell g_{\ell+1} + \alpha_\ell g_\ell + \beta_\ell = 0, \quad \ell = n,\dots,2,1. \tag{13b}$$

Applying (13a) and (13b) to (12), we can show that $\beta_i p_{i-1,j} + \alpha_i p_{ij} + \gamma_i p_{i+1,j} = 0$ in (11) if $i \neq j$. This leads to $s_{ij} = 0$ for $i \neq j$. Therefore, it is proved that $s_{ij} = 1$ if $i = j$ and $s_{ij} = 0$ otherwise. □

Theorem 1 does not state a relationship between p_{ij} and p_{ji}. To clarify this point and supplement how v_{ji} is related to v_{ij}, we provide the following lemma.

LEMMA 2. *The product integrals p_{ij} and p_{ji} defined by (4) are connected with*

$$p_{ji} = \begin{cases} p_{ij} \dfrac{v_{ii}}{v_{jj}} \prod_{\ell=i}^{j-1} \dfrac{\beta_{\ell+1}}{\gamma_\ell} & \text{if } i < j \\ p_{ij} \dfrac{v_{jj}}{v_{ii}} \prod_{\ell=j}^{i-1} \dfrac{\gamma_\ell}{\beta_{\ell+1}} & \text{if } j < i \end{cases}.$$

Lemma 2 is motivated easily by Usmani's result [16]. A proof of Lemma 2 can be immediately completed using [16, Section 4], provided Theorem 1 is true. However, to see a simple proof, here we prove Lemma 2 independently of these results.

Proof of Lemma 2. First, for simplicity, we will show that

$$\frac{v_{i+1,i+1}}{v_{ii}} = \frac{f_i}{g_{i+1}} \frac{\beta_{i+1}}{\gamma_i},$$

which is the case of $j = i+1$ in this lemma because of (4’). This equation is demonstrated as follows:

$$\begin{aligned} & g_{i+1} v_{i+1,i+1} \gamma_i - f_i v_{ii} \beta_{i+1} \\ & \quad = g_{i+1}\{f_i \beta_{i+1} + \alpha_{i+1} + g_{i+2}\gamma_{i+1}\}\gamma_i - f_i\{f_{i-1}\beta_i + \alpha_i + g_{i+1}\gamma_i\}\beta_{i+1} \ \ (\text{using } (5')) \\ & \quad = \{g_{i+1} f_i \beta_{i+1} - \beta_{i+1}\}\gamma_i - \{-\gamma_i + f_i g_{i+1}\gamma_i\}\beta_{i+1} \ (\text{by } (13a), (13b)) \\ & \quad = 0. \end{aligned}$$

Since an arbitrary i can be replaced by $i+\xi$ $(\xi \geqslant 1)$, we also have

$$\frac{v_{i+\xi+1,i+\xi+1}}{v_{i+\xi,i+\xi}} = \frac{f_{i+\xi}\beta_{i+\xi+1}}{g_{i+\xi+1}\gamma_{i+\xi}} \quad \text{for } \xi \geqslant 0. \tag{14}$$

Hence, repeatedly using (14) if $i < j$, part of this lemma can be shown as

$$\frac{v_{jj}}{v_{ii}} = \frac{v_{i+1,i+1}}{v_{ii}} \frac{v_{i+2,i+2}}{v_{i+1,i+1}} \cdots \frac{v_{jj}}{v_{j-1,j-1}} = \prod_{\xi=0}^{j-i-1} \frac{f_{i+\xi}\beta_{i+\xi+1}}{g_{i+\xi+1}\gamma_{i+\xi}} = \frac{p_{ij}}{p_{ji}} \prod_{\ell=i}^{j-1} \frac{\beta_{\ell+1}}{\gamma_\ell}.$$

Using a similar method, the results in the case of $j < i$ can be also demonstrated. Then, for example, we can show

$$\frac{v_{i-\eta-1,i-\eta-1}}{v_{i-\eta,i-\eta}} = \frac{g_{i-\eta}\gamma_{i-\eta-1}}{f_{i-\eta-1}\beta_{i-\eta}} \text{ for } \eta \geqslant 0. \tag{15}$$

A more immediate proof of (15) is achieved by replacing i in (14) with j. □

The following lemma gives the relationship between f_ℓ, g_ℓ and minors, which clarifies how Theorem 1 is related to the Usmani formula.

LEMMA 3. *f_ℓ and g_ℓ are related to the minors θ_ℓ and ϕ_ℓ as follows*

$$f_\ell = -\gamma_\ell \frac{\theta_{\ell-1}}{\theta_\ell} \text{ and } g_\ell = -\beta_{\ell+1}\frac{\phi_{\ell+1}}{\phi_\ell}. \tag{16}$$

Proof of Lemma 3. We can translate the relation $\theta_\ell = \alpha_\ell\theta_{\ell-1} - \gamma_{\ell-1}\beta_\ell\theta_{\ell-2}$ as follows

$$\frac{1}{\frac{\theta_\ell}{\theta_{\ell-1}}} = \frac{1}{\alpha_\ell - \gamma_{\ell-1}\beta_\ell\frac{\theta_{\ell-2}}{\theta_{\ell-1}}} \Rightarrow \; -\gamma_\ell\frac{\theta_{\ell-1}}{\theta_\ell} = \frac{-\gamma_\ell}{\alpha_\ell + \beta_\ell\left(-\gamma_{\ell-1}\frac{\theta_{\ell-2}}{\theta_{\ell-1}}\right)},$$

which yields (3a) using (16). Also, the relation $\phi_\ell = \alpha_\ell\phi_{\ell+1} - \gamma_\ell\beta_{\ell+1}\phi_{\ell+2}$ can be translated to

$$\frac{1}{\frac{\phi_\ell}{\phi_{\ell+1}}} = \frac{1}{\alpha_\ell - \gamma_\ell\beta_{\ell+1}\frac{\phi_{\ell+2}}{\phi_{\ell+1}}} \Rightarrow \; -\beta_{\ell+1}\frac{\phi_{\ell+1}}{\phi_\ell} = \frac{-\beta_{\ell+1}}{\alpha_\ell + \gamma_{\ell+1}\left(-\beta_{\ell+1}\frac{\theta_{\ell+2}}{\theta_{\ell+1}}\right)} \Rightarrow \text{(3b)}. \quad \square$$

Proof of Corollary 1. Note that a matrix expression of Z_n is $Z_n = Q_nT_nQ_n$ in Corollary 1, where

$$Q_n = \operatorname{diag}(q_1,\dots,q_n),\; T_n = \begin{pmatrix} \tau_1 & \cdots & \tau_1 & \tau_1 \\ \vdots & \ddots & & \\ \tau_1 & & \tau_{n-1} & \tau_{n-1} \\ \tau_1 & & \tau_{n-1} & \tau_n \end{pmatrix} \text{ and } \tau_j = \sum_{\ell=1}^{j}\frac{\mu_\ell}{r_\ell(r_\ell-\mu_\ell)}.$$

Let $\rho_i = 1/(\tau_i - \tau_{i-1})$. The inverse of T_n with a martingale covariance structure is the following tridiagonal matrix

$$T_n^{-1} = \begin{pmatrix} \rho_1+\rho_2 & -\rho_2 & 0 & \cdots & 0 \\ -\rho_2 & \rho_2+\rho_3 & -\rho_2 & \ddots & \vdots \\ 0 & -\rho_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \rho_{n-1}+\rho_n & -\rho_n \\ 0 & \cdots & 0 & -\rho_n & \rho_n \end{pmatrix}.$$

Then, by the relations $1-q_{i-1}/q_i = -\mu_i/(r_i-\mu_i)$ and $1-q_i/q_{i-1} = \mu_i/r_i$, we have

$$\rho_i = \mu_i\left(\frac{r_i}{\mu_i}\right)^2\left(1-\frac{\mu_i}{r_i}\right) = \mu_i\left(1-\frac{q_i}{q_{i-1}}\right)^{-2}\left(\frac{q_i}{q_{i-1}}\right) = q_{i-1}q_i\frac{\mu_i}{(q_i-q_{i-1})^2}.$$

Using this result and the above relations, we further obtain

$$\rho_i+\rho_{i+1}-q_i^2\left\{\frac{\mu_i}{(q_i-q_{i-1})^2}+\frac{\mu_{i+1}}{(q_{i+1}-q_i)^2}\right\} = -\frac{\mu_i}{(1-q_{i-1}/q_i)}+\frac{\mu_{i+1}}{(q_{i+1}/q_i-1)} = \delta_i.$$

Therefore, we can show that $Z_n^{-1} = Q_n^{-1}T_n^{-1}Q_n^{-1}$ is equal to Y_n. $\square$

4. A study of the limit of an inverse matrix

EXAMPLE 1. Consider the limit form of the inverse of

$$Y_n = \begin{pmatrix} 2n+c_n & -n & 0 & \cdots & 0 \\ -n & 2n+c_n & -n & \ddots & \vdots \\ 0 & -n & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -n \\ 0 & \cdots & 0 & -n & 2n+c_n \end{pmatrix} \quad \text{for some } c_n > 0.$$

A stationary case of (3a) and (3b) gives the equation

$$x^{(n)} = \frac{n}{-nx^{(n)}+2n+c_n}$$

whose solutions $x_1^{(n)}$ and $x_2^{(n)}$ are

$$x_1^{(n)} = (2n+c_n+\sqrt{c_n(4n+c_n)})/2n \text{ and } x_2^{(n)} = (2n+c_n-\sqrt{c_n(4n+c_n)})/2n.$$

Throughout this section, let a and b be constants bounded away from 0 and 1 and independent of n, and put $i = \lfloor an \rfloor$ and $j = \lfloor bn \rfloor$, where $\lfloor u \rfloor$ is the largest integer not greater than u. Then, as $n \to \infty$, f_i and g_i converge to $x_1^{(\infty)}$ (i.e., the limit of $x_1^{(n)}$) satisfying

$$f_\ell = \frac{\{x_1^{(n)}\}^\ell - \{x_2^{(n)}\}^\ell}{\{x_1^{(n)}\}^{\ell+1} - \{x_2^{(n)}\}^{\ell+1}} \quad \text{and} \quad g_\ell = \frac{\{x_1^{(n)}\}^{n-\ell+1} - \{x_2^{(n)}\}^{n-\ell+1}}{\{x_1^{(n)}\}^{n-\ell+2} - \{x_2^{(n)}\}^{n-\ell+2}}, \tag{17}$$

$\ell = 1,2,\ldots,n$, by Binet's formula (see [16, Section 3]). Based on these results, we can study the limits of v_{ij} and z_{ij}. Assume $c_n = c^2/n$ for some c independent of n. Then, according to (17), we can show

$$\begin{aligned} \lim_{n\to\infty} n(1-f_{nt-1}) &= \lim_{n\to\infty} n\left(1-\frac{x_1^{(n)nt-1}-x_2^{(n)nt-1}}{x_1^{(n)nt}-x_2^{(n)nt}}\right) = \lambda(t;c), \\ \lim_{n\to\infty} n(1-g_{n(1-s)+1}) &= \lim_{n\to\infty} n\left(1-\frac{x_1^{(n)ns}-x_2^{(n)ns}}{x_1^{(n)ns+1}-x_2^{(n)ns+1}}\right) = \lambda(s;c) \end{aligned} \tag{18}$$

for t and $1-s$ between a and b, where $\lambda(t;c)=c(\mathrm{e}^{2ct}+1)/(\mathrm{e}^{2ct}-1)$. Hence, we have

$$\begin{aligned}\lim_{n\to\infty} v_{jj} &= \lim_{n\to\infty}\left(n(1-f_{j-1})+c^2/n+n(1-g_{j+1})\right) \text{ from } (5')\\ &= \lambda(b;c)+\lambda(1-b;c)\end{aligned}$$

using (18). Further, we obtain

$$\lim_{n\to\infty} p_{ij} = \begin{cases} \text{if } i\leqslant j,\ \exp\left\{-\lim_{n\to\infty}\int_a^b n(1-f_{nt})dt\right\} \\ \text{if } i>j,\ \exp\{-\lim_{n\to\infty}\int_{1-a}^{1-b} n(1-g_{n(1-s)})ds\}\end{cases} = \begin{cases}\exp\left(-\int_a^b \lambda(t;c)dt\right)\\ \exp(-\int_{1-a}^{1-b}\lambda(s;c)ds)\end{cases}$$

because, e.g. if $i<j$, we have

$$\lim_{n\to\infty}\prod_{\ell=i}^{j-1} f_\ell = \lim_{n\to\infty}\exp\{-n^{-1}\sum_{\ell=i}^{j-1} n(1-f_\ell)\} = \lim_{n\to\infty}\exp\left\{-\int_a^b n(1-f_{nt})dt\right\}$$

by the property of the product integral based on (4) and $f_\ell\to 1$. Thus, we conclude that

$$\lim_{n\to\infty} z_{ij} = \lim_{n\to\infty}\frac{p_{ij}}{v_{jj}} = \begin{cases}\exp(-\int_a^b\lambda(t;c)dt)/\{\lambda(b;c)+\lambda(1-b;c)\} & \text{if } a\leqslant b,\\ \exp(-\int_b^a\lambda(1-t;c)dt)/\{\lambda(b;c)+\lambda(1-b;c)\} & \text{if } a>b.\end{cases}$$

EXAMPLE 2. Extending Example 1, we discuss the inverse of

$$Y_n = \begin{pmatrix} n(d_0^2+d_1^2)+c_1^2/n & -nd_1^2 & 0 & \cdots & 0\\ -nd_1^2 & n(d_1^2+d_2^2)+c_2^2/n & -nd_2^2 & \ddots & \vdots\\ 0 & -nd_2^2 & \ddots & \ddots & 0\\ \vdots & \ddots & \ddots & \ddots & -nd_{n-1}^2\\ 0 & \cdots & 0 & -nd_{n-1}^2 & n(d_{n-1}^2+d_n^2)+c_n^2/n\end{pmatrix}.$$

Suppose that d_ℓ's and c_ℓ's are discrete approximations of continuous functions $d(t)$ and $c(t)$ on $t\in[0,1]$ such that $d_\ell=d(\ell/n)$ and $c_\ell=c(\ell/n)$, where $d(t)$ is bounded away from zero. Referring to Example 1, let $S_f(b;a)=\exp(-\int_a^b\lim_{n\to\infty} n(1-f_{nt})dt)$ and $S_g(b;a)=\exp(-\int_b^a\lim_{n\to\infty} n(1-g_{nt})dt)$. These are the limit forms of p_{ij} (for $i=\lfloor an\rfloor$, $j=\lfloor bn\rfloor$) if Lebesgue's convergence theorem can be applied to integrals of $n(1-f_{nt})$ and $n(1-g_{nt})$. Using Theorem 1, as n is larger, we can examine computationally how $n(1-f_{nt})$ and $n(1-g_{nt})$ behave in order to know a domain of a and b in which p_{ij} can be well approximated by $S_f(b;a)$ or $S_g(b;a)$. On the other hand, even if the limits of $n(1-f_{nt})$ and $n(1-g_{nt})$ produced by non-constant $d(t)$ and $c(t)$ are expressed using some well-known functions, it may be difficult in many cases that the corresponding $S_f(b;a)$ and $S_g(b;a)$ have the closed forms. However, we can still investigate $S_f(b;a)$, $S_g(b;a)$ and limits of z_{ij} computationally using p_{ij} or a numerical integration. For limits of diagonal z_{ii}, it is necessary only to evaluate $n(1-f_{na})$ and $n(1-g_{na})$. We consider an approach to evaluate limits of $n(1-f_{nt})$ and $n(1-g_{nt})$ below.

Stationary cases of (3a) and (3b) give the equations of $x^{(n)}_{\ell/m}$,

$$x^{(n)}_{\ell/m} = \frac{d(\ell_0/m)^2}{-d(\ell_1/m)^2 x^{(n)}_{\ell/m} + \{d((\ell-1)/m)^2 + d(\ell/m)^2\} + c(\ell/m)^2/n^2}$$

under $m = n$, where $(\ell_0, \ell_1) = (\ell, \ell-1)$ in the case of (3a) and $(\ell_0, \ell_1) = (\ell-1, \ell)$ in (3b). Let $x^{(n)_h}_{\ell/m,1}$ and $x^{(n)_h}_{\ell/m,2}$, $h = f, g$ be the above solutions

$$2^{-1} d(\ell_h/m)^{-2}\Big[d((\ell-1)/m)^2 + d(\ell/m)^2 + c(\ell/m)^2/n^2 \\ \pm\sqrt{\{d((\ell-1)/m)^2 + d(\ell/m)^2 + c(\ell/m)^2/n^2\}^2 - 4d((\ell-1)/m)^2 d(\ell/m)^2}\Big]$$

and assume $x^{(n)_h}_{\ell/m,1} > x^{(n)_h}_{\ell/m,2}$, where $\ell_f = \ell - 1$ and $\ell_g = \ell$. To separate m and n formally, we introduce a function $\varepsilon(t)$ such that

$$d((\ell-1)/m) = d(\ell/m) - \varepsilon(\ell/m)/n. \tag{19}$$

In addition, letting $f^{(\ell/m)}_\ell = f_\ell$ and $g^{(\ell/m)}_\ell = g_\ell$, as $m \to \infty$ and $\ell/m \to t$, consider the sequences $f^{(t)}_i$ and $g^{(t)}_i$ which follow Binet's formula

$$\lim_{m\to\infty} f^{(\ell/m)}_i = \frac{\{x^{(n)_f}_{t,1}\}^i - \{x^{(n)_f}_{t,2}\}^i}{\{x^{(n)_f}_{t,1}\}^{i+1} - \{x^{(n)_f}_{t,2}\}^{i+1}}$$

$$\text{and} \quad \lim_{m\to\infty} g^{(\ell/m)}_i = \frac{\{x^{(n)_g}_{t,1}\}^{n-i+1} - \{x^{(n)_g}_{t,2}\}^{n-i+1}}{\{x^{(n)_g}_{t,1}\}^{n-i+2} - \{x^{(n)_g}_{t,2}\}^{n-i+2}}.$$

By taking $\lim_n$ into the both sides, we have

$$\lim_{n\to\infty} n(1 - f^{(t)}_{nt}) = \lambda_f(t; c, d, \varepsilon) = A(t)\left(\frac{e^{2A(t)t} + 1}{e^{2A(t)t} - 1}\right) + \frac{\varepsilon(t)}{d(t)}$$

$$\text{and} \quad \lim_{n\to\infty} n(1 - g^{(t)}_{nt}) = \lambda_g(1-t; c, d, \varepsilon) = A(t)\left(\frac{e^{2A(t)(1-t)} + 1}{e^{2A(t)(1-t)} - 1}\right) - \frac{\varepsilon(t)}{d(t)},$$

where $A(t) = \sqrt{d(t)^2(c(t)^2 + \varepsilon(t)^2)}/d(t)^2$. Hence, using the epsilon-delta proof, we can show that $\lim_{n=m\to\infty} n(1 - f_{nt})$ exists and is $\lambda_f(t; c, d, \varepsilon)$, because

$$\lim_{n\to\infty}\lim_{m\to\infty} n(1 - f^{(\ell/m)}_{nt}) \text{ and } \lim_{m\to\infty} n(1 - f^{(\ell/m)}_{nt}) \text{ do exist.}$$

Also, a similar discussion leads to $\lim_{n=m\to\infty} n(1 - g_{nt}) = \lambda_g(1-t; c, d, \varepsilon)$. Therefore, under these settings, for $i = \lfloor an \rfloor$ and $j = \lfloor bn \rfloor$, it is obtained that

$$\lim_{n\to\infty} z_{ij} = \begin{cases} S_f(b;a)/\left[d(b)^2\{\lambda_f(b; c, d, \varepsilon) + \lambda_g(1-b; c, d, \varepsilon)\}\right] & \text{if } a \leqslant b, \\ S_g(b;a)/\left[d(b)^2\{\lambda_f(b; c, d, \varepsilon) + \lambda_g(1-b; c, d, \varepsilon)\}\right] & \text{if } a > b. \end{cases}$$

The important problem still left here is how to determine $\varepsilon(t)$, but this is not provided in this paper (however, if we consider the case of Example 3, $\varepsilon(t)$ can be analyzed at least using (20)). Generally, it is not true that $\varepsilon(t)$ is the first derivative $d'(t)$ of $d(t)$, because (19) is not a complete equation to determine $\varepsilon(\cdot)$ and, for example, some dependence between m and n to justify the above-mentioned two step of limit operations is required in addition to (19). However, if all d_ℓ's are constant, we can say $\varepsilon(t)=0$. We tried many cases of $d(t)$ and $c(t)$, so that $n(1-f_{nt})$ was observed between $\lambda_f(t;c,d,\varepsilon)|_{\varepsilon(t)=-d'(t)}$ and $\lambda_f(t;c,d,\varepsilon)|_{\varepsilon(t)=0}$ (similarly, $n(1-g_{nt})$ was between $\lambda_g(1-t;c,d,-d')$ and $\lambda_g(1-t;c,d,0)$).

EXAMPLE 3 (Numerical experiment). We here perform a numerical experiment to invert a symmetric tridiagonal matrix ($\gamma_i=\beta_{i+1}$). The performance of Theorem 1 is compared with the LU factorization methods [3, 1] and the cyclic reduction method [9] freed of determinant expressions. For this experiment, we create a case where the limit of z_{ij} is known using Corollary 1. Let $\{h_\ell\}_{\ell=1}^n$ and $\{r_\ell\}_{\ell=1}^n$ be discrete approximations of continuous functions $h(t)$ and $r(t)$ on $[0,1]$ such that $h_\ell=h(\ell/n)$ and $r_\ell=r(\ell/n)$. Put $r_{n+1}=0$,

$$\mu_i=n^{-1}h_ir_i \text{ and } \delta_i=(r_i-r_{i+1})-\mu_i,\ i=1,\dots,n,$$

and then the sequences $\{\alpha_i\}_{i=1}^n$ and $\{\beta_i\}_{i=2}^n$ are obtained from (6), where

$$q_i=\textstyle\prod_{\ell=1}^i(1-h_\ell/n).$$

Since we have $z_{ij}=q_iq_j\sum_{\ell=1}^{\min(i,j)}n^{-1}h_\ell/(r_\ell-\mu_\ell)$ applying Corollary 1 to Y_n made like this, we can obtain the limit form of z_{ij} for $i=\lfloor an\rfloor$ and $j=\lfloor bn\rfloor$

$$\lim_{n\to\infty}z_{ij}=q(a)q(b)\int_0^{\min(a,b)}\frac{h(t)}{r(t)}dt,\quad \text{where } q(t)=\exp(-\textstyle\int_0^t h(s)ds). \tag{20}$$

Let z_{ij}^{P}, z_{ij}^{C}, z_{ij}^{A} and z_{ij}^{E} be numerical values of z_{ij} computed by the methods of Theorem 1, the cyclic reduction, [1] and [3], respectively. All algorithms for these methods are written in the Fortran language, and Compaq Visual Fortran 6.5 is used as the compiler. For the cyclic reduction method, the subroutine `DSLR` of the IMSL library is used. Considering the patterns of $n=500$, 1000, 2000, 5000 and 10000, we observe computational times (until $z_{ij}^{\mathscr{M}}$, $i,j=1,\dots,n$ are obtained) and the following numerical errors

$$\begin{aligned} SE^{\mathscr{M}} &= \textstyle\sum_{i=1}^n\sum_{j=1}^n\{\log(z_{ij}^{\mathscr{M}}/z_{ij}^{(\infty)})\}^2,\\ AE^{\mathscr{M}} &= \sup_{i,j=1,\dots,n}|\log(z_{ij}^{\mathscr{M}}/z_{ij}^{(\infty)})|,\quad \mathscr{M}=\mathrm{P,C,A,E}, \end{aligned}$$

where $z_{ij}^{(\infty)}=q(i/n)q(j/n)\int_0^{\min(i/n,j/n)}h(t)r(t)^{-1}dt$ from (20).

We provide the result of this experiment when $h(t)=1+\cos(2\pi t)$ and $r(t)=1$ in Table 1, where the computation for [3] was stopped when $n=5000$ and 10000, because the computational time was too long. This result shows that the method of Theorem 1 has a faster computation than not only the LU factorization methods, but

Table 1: *Result of the numerical experiment when* $h(t) = 1 + \cos(2\pi t)$ *and* $r(t) = 1$.

Method: $\mathscr{M}$		n = 500	1000	2000	5000	10000
Times (sec.)	P	0.6	7.7	13.4	61.7	257.6
	C	1.8	4.7	18.7	116.0	465.8
	A	1.3	5.0	24.9	291.7	2114.8
	E	184	2908	46258	–	–
$SE^{\mathscr{M}}$	P	7.47×10^{-20}	2.94×10^{-17}	0.78×10^{-16}	5.91×10^{-10}	0.65×10^{-12}
	C	10.7×10^{-20}	0.45×10^{-17}	7.72×10^{-16}	5.84×10^{-10}	2.92×10^{-12}
	A	0.25×10^{-20}	6.67×10^{-17}	2.91×10^{-16}	5.80×10^{-10}	10.7×10^{-12}
	E	1.22×10^{-20}	2.15×10^{-17}	4.18×10^{-16}	–	–
$AE^{\mathscr{M}}$	P	12.6×10^{-13}	7.26×10^{-12}	0.97×10^{-11}	5.55×10^{-9}	1.69×10^{-10}
	C	8.58×10^{-13}	2.96×10^{-12}	1.63×10^{-11}	5.51×10^{-9}	2.01×10^{-10}
	A	3.13×10^{-13}	9.43×10^{-12}	1.05×10^{-11}	5.49×10^{-9}	3.61×10^{-10}
	E	3.69×10^{-13}	5.31×10^{-12}	1.16×10^{-11}	–	–

the cyclic reduction method if n is sufficiently large. However, in the two numerical errors, the method of Theorem 1 are not inferior to the LU factorization methods and the cyclic reduction method. Similar tendency to Table 1 is obtained for the other functions of $h(t)$ and $r(t)$. For these experiments we used a computer with an Intel Core2 Quad processor with 3GHz and with 8GBytes of main memory.

5. Remark in the case of zero minors

GENERAL. Theorem 1 usually gives a stable computation, but a number of points must be dealt with cautiously when minors θ_η or ϕ_ξ are zeros. Consider the case of

$$f_{\eta-1}\beta_\eta + \alpha_\eta = 0,\ \eta \in \mathcal{I}, \tag{21a}$$

$$\text{and/or} \quad g_{\xi+1}\gamma_\xi + \alpha_\xi = 0,\ \xi \in \mathcal{J}, \tag{21b}$$

where $\mathcal{I}$ and $\mathcal{J}$ are subsets of indices $\{1,\dots,n\}$.

LEMMA 4. *For $\eta \in \mathcal{I}$ and $\xi \in \mathcal{J}$, (21a) and (21b) are equivalent to $\theta_\eta = 0$ and $\phi_\xi = 0$, respectively. Condition (21a) under $\theta_n \neq 0$ provides $\gamma_\eta \neq 0$, $\beta_{\eta+1} \neq 0$, $\phi_{\eta+2} \neq 0$, $\theta_{\eta-1} \neq 0$ and $\theta_{\eta+1} \neq 0$. Also, (21b) under $\theta_n \neq 0$ leads to $\gamma_{\xi-1} \neq 0$, $\beta_\xi \neq 0$, $\theta_{\xi-2} \neq 0$, $\phi_{\xi-1} \neq 0$ and $\phi_{\xi+1} \neq 0$.*

Proof of Lemma 4. By (21a) and Lemma 3, we have

$$f_{\eta-1} = -\alpha_\eta/\beta_\eta = -\gamma_{\eta-1}\theta_{\eta-2}/\theta_{\eta-1}.$$

This leads to $\theta_\eta = \alpha_\eta \theta_{\eta-1} - \beta_\eta \gamma_{\eta-1} \theta_{\eta-2} = 0$. Similarly, $\phi_\xi = 0$ can be shown by (21b) and Lemma 3. In addition, any of $\gamma_\eta = 0$, $\beta_{\eta+1} = 0$ or $\phi_{\eta+2} = 0$ under $\theta_\eta = 0$ provides $\theta_n = 0$ by [16, (1.5)]. Similarly, $\phi_\xi = 0$ and $\theta_n \neq 0$ result in $\gamma_{\xi-1} \neq 0$, $\beta_\xi \neq 0$ and $\theta_{\xi-2} \neq 0$. The conditions $\theta_{\eta-1} \neq 0$, $\theta_{\eta+1} \neq 0$, $\phi_{\xi-1} \neq 0$ and $\phi_{\xi+1} \neq 0$ hold clearly by [16, Lemma 1]. □

Suppose (21a) and/or (21b) (i.e. $\theta_\eta = 0$ and/or $\phi_\xi = 0$). Simultaneously, $\gamma_\eta \neq 0$, $\beta_{\eta+1} \neq 0$ and $\phi_{\eta+2} \neq 0$, and/or $\gamma_{\xi-1} \neq 0$, $\beta_\xi \neq 0$ and $\theta_{\xi-2} \neq 0$ are assumed according to Lemma 4. For simplicity, we set $\theta_\ell \neq 0$, $\ell \leqslant \eta - 1$ and $\phi_\ell \neq 0$, $\ell \geqslant \xi + 1$ in the following contents. By Lemma 4, (21a) means that $|f_\eta| = \infty$ and $f_{\eta+1} = 0$, which provides

$$f_\eta f_{\eta+1} = -\frac{\gamma_{\eta+1}}{\beta_{\eta+1} + \alpha_{\eta+1}/f_\eta} \to -\frac{\gamma_{\eta+1}}{\beta_{\eta+1}} \text{ as } |f_\eta| \to \infty.$$

Similarly, (21b) leads to $|g_\xi| = \infty$ and $g_{\xi-1} = 0$, which provides

$$g_{\xi-1} g_\xi = -\frac{\beta_{\xi-1}}{\gamma_{\xi-1} + \alpha_{\xi-1}/g_\xi} \to -\frac{\beta_{\xi-1}}{\gamma_{\xi-1}} \text{ as } |g_\xi| \to \infty.$$

Hence, p_{ij} is computed as

$$p_{ij} = \begin{cases} p_{i\eta} f_\eta = \pm\infty & \text{if } j = \eta+1,\ i < j \\ p_{i\eta}\left(-\gamma_{\eta+1}/\beta_{\eta+1}\right) p_{\eta+2,j} & \text{if } j \geqslant \eta+2,\ i < j \\ g_\xi p_{i\xi} = \pm\infty & \text{if } j = \xi - 1,\ i > j \\ p_{\xi-2,j}\left(-\beta_{\xi-1}/\gamma_{\xi-1}\right) p_{i\xi} & \text{if } j \leqslant \xi - 2,\ i > j \end{cases} \tag{22}$$

and as usual otherwise (i.e. $j \leqslant \eta$ and $i \leqslant j$ or $j \geqslant \xi$ and $i \geqslant j$), satisfying $p_{ii} = 1$. Therefore, if $j \neq \eta + 1$ or $j \neq \xi - 1$, z_{ij} is computed by $z_{ij} = p_{ij}/v_{jj}$, using p_{ij} of (22); otherwise this is

$$z_{ij} = \begin{cases} 0 & \left(= \frac{1}{\beta_{\eta+1} f_\eta + \alpha_{\eta+1} + \gamma_\eta g_{\eta+2}}\right) \text{ if } j = \eta+1 \text{ and } i = j \\ p_{i\eta}/\beta_{\eta+1} & \left(= \frac{p_{i\eta} f_\eta}{\beta_{\eta+1} f_\eta + \alpha_{\eta+1} + \gamma_\eta g_{\eta+2}}\right) \text{ if } j = \eta+1 \text{ and } i < j \\ 0 & \left(= \frac{1}{\beta_{\xi-1} f_{\xi-2} + \alpha_{\xi-1} + \gamma_{\xi-1} g_\xi}\right) \text{ if } j = \xi-1 \text{ and } i = j \\ p_{i\xi}/\gamma_{\xi-1} & \left(= \frac{g_\xi p_i^{(\xi)}}{\beta_{\xi-1} f_{\xi-2} + \alpha_{\xi-1} + \gamma_{\xi-1} g_\xi}\right) \text{ if } j = \xi-1 \text{ and } i > j \end{cases} \tag{23}$$

by $z_{i,\eta+1} = \lim_{|f_\eta| \to \infty} p_{i,\eta+1}/v_{\eta+1,\eta+1}$ and $z_{i,\xi-1} = \lim_{|g_\xi| \to \infty} p_{i,\xi-1}/v_{\xi-1,\xi-1}$.

A NUMERICAL EXAMPLE. As a numerical example of Theorem 1, we consider the inverse of the matrix

$$Y_6 = \begin{pmatrix} 2 & 1 & 0 & 0 & 0 & 0 \\ -1 & -2 & \sqrt{3} & 0 & 0 & 0 \\ 0 & -\sqrt{3} & 2 & 2 & 0 & 0 \\ 0 & 0 & -1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{pmatrix}.$$

A special feature of Y_6 is that the minor $\theta_3 = 0$. This leads to $f_2\beta_3 + \alpha_3 = 0$, which gives $f_3 = -\infty$, $\mathcal{I} = \{3\}$ and $\mathcal{J} = \{\emptyset\}$. It is easy to verify that

$$(f_1, f_2, f_3, f_4, f_5) = \left(-1/2, 2/\sqrt{3}, -\infty, 0, -1\right),$$
$$(g_2, g_3, g_4, g_5, g_6) = \left(-1, 1/\sqrt{3}, 1/2, 0, 1/2\right).$$

Therefore, noting that $-\gamma_4/\beta_4 = 1$ and the zero-minors version (22) of (4), the matrix expression of p_{ij} is

$$(p_{ij})_{i,j=1}^{6} = \begin{pmatrix} 1 & -1/2 & -1/\sqrt{3} & \infty & -1/\sqrt{3} & 1/\sqrt{3} \\ -1 & 1 & 2/\sqrt{3} & -\infty & 2/\sqrt{3} & -2/\sqrt{3} \\ -1/\sqrt{3} & 1/\sqrt{3} & 1 & -\infty & 1 & -1 \\ -1/2\sqrt{3} & 1/2\sqrt{3} & 1/2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 1/2 & 1 \end{pmatrix},$$

while the list of v_{jj} is

$$\begin{aligned} v_{11} &= 2 + g_2 = 1, & v_{44} &= -f_3 - 2 + g_5 = \infty, \\ v_{22} &= -f_1 - 2 + \sqrt{3}g_3 = -\frac{1}{2}, & v_{55} &= 0f_4 + 2 + 2g_6 = 3 \\ v_{33} &= -\sqrt{3}f_2 + 2 + 2g_4 = 1, & v_{66} &= -f_5 + 2 = 3. \end{aligned}$$

Using Theorem 1 and its zero-minors version (23) applied to the case of $\eta = 3$, we have

$$Z_6 = \begin{pmatrix} 1 & 1 & -1/\sqrt{3} & 1/\sqrt{3} & -1/3\sqrt{3} & 1/3\sqrt{3} \\ -1 & -2 & 2/\sqrt{3} & -2/\sqrt{3} & 2/3\sqrt{3} & -2/3\sqrt{3} \\ -1/\sqrt{3} & -2/\sqrt{3} & 1 & -1 & 1/3 & -1/3 \\ -1/2\sqrt{3} & -1/\sqrt{3} & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/3 & -1/3 \\ 0 & 0 & 0 & 0 & 1/6 & 1/3 \end{pmatrix}.$$

This example shows that we can have infinite values in the intermediate computations without symbolic handling such as Algorithm 2 of [7]. If we apply the algorithm in the floating point arithmetic that supports IEEE standards which can handle ∞, the automatic computation will be performed.

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