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A NOTE ON THE INVERSION OF ACYCLIC MATRICES

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Abstract: Our goal is to generalize some well known results on the inversion of nonsingular tridiagonal matrices to matrices whose graph is a given tree, bringing the results together in one place. A numerical example and a statistical application are given.

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1. Introduction

Inversion of tridiagonal or Jacobi matrices is a fairly popular field in pure and applied mathematics. This subject has many engineering applications and it lies at the crossroads of physics, chemistry, linear algebra, differential equations, approximation theory, statistics, numerical analysis and, also, graph theory.

Historically, Moskovitz [25] in 1944 first gave an explicit formula for the inverse of a tridiagonal matrix related one dimensional and two dimensional Poisson problems. Though, earlier in 1937, Gantmacher and Krein [13] proved with some explicit calculations that the inverse of a symmetric Jacobi matrix is a one-pair matrix. In 1953, Berger and Saibel [6] provided an explicit formula for calculating the inverse of a continuant matrix, based on the LU-decomposition with no conditions on the elements of the continuant matrix. They also provided some conditions for the inverse of a continuant matrix to have "gnomonic symmetry". Later on, Roy and Sarhan [26] inverted very spe-

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cific matrices arising in statistical applications, and S.O. Asplund, proved in [2] the same as Gantmacher and Krein, by calculating the inverse via techniques for solving finite boundary value problems. A brief remark states that higher order band matrices have as inverses higher order Green's matrices. Since then most the results that have been obtained are quite often unrelated.

Consider the tridiagonal matrix of order n

$$A = \begin{pmatrix} a_1 & b_1 & & & \\ c_1 & a_2 & b_2 & & \\ & c_2 & \ddots & \ddots & \\ & & \ddots & \ddots & b_{n-1} \\ & & & c_{n-1} & a_n \end{pmatrix} . \tag{1.1}$$

In [27] Schlegel gave a closed form inverse of the matrix (1.1) when $b_i = c_i = 1$ and $a_i = a_{n-i+1}$, a slight generalization of a matrix considered by Kershaw [19]. In the case of a integer matrix, the inverse can be computed without machine roundoff error.

For the general case, suppose now that all the c_i's are nonzero and define $\mu_n = 1$, $\mu_{n-1} = -f_n$ and

$$\mu_i = -f_{i+1}\mu_{i+1} - g_{i+1}\mu_{i+2} \,,$$

where

$$f_i = \frac{a_i}{c_{i-1}} \quad \text{and} \quad g_i = \frac{b_i}{c_{i-1}} \,.$$

Lewis [20] proved that A defined in (1.1) is nonsingular if and only if $a_1\mu_1 + b_1\mu_2 \neq 0$. In this case if one defines $A^{-1} = (\alpha_{ij})$, then, for $i \geq j$,

$$\alpha_{ij} = \mu_i \alpha_{nj} \,, \quad \text{with} \quad \alpha_{n1} = (a_1\mu_1 + b_1\mu_2)^{-1}$$

and

$$\alpha_{nj} = \begin{cases} \dfrac{b_{j-1}\mu_j\alpha_{nj-1} - 1}{c_{j-1}\mu_{j-1}} \,, & \text{if } \mu_{j-1} \neq 0 \,, \\ -\dfrac{b_{j-2}\alpha_{nj-2} + a_{j-1}\alpha_{nj-1}}{c_{j-1}} \,, & \text{if } \mu_{j-1} = 0 \,. \end{cases}$$

In the case $i < j$,

$$\alpha_{ij} = \alpha_{ji} \prod_{k=i}^{j-1} \frac{b_k}{c_k} \,.$$

An alternative approach was given in [30]. Usmani considered the sequences $\theta_0, \theta_1, \ldots, \theta_n$ defined by the three-term recurrence relation

$$\theta_0 = 1 \ , \quad \theta_1 = a_1 \ , \quad \theta_i = a_i\theta_{i-1} - b_{i-1}c_{i-1}\theta_{i-2} \ , \tag{1.2}$$

and $\phi_1, \ldots, \phi_n, \phi_{n+1}$, defined by the three-term recurrence relation

$$\phi_{n+1} = 1 \ , \quad \phi_n = a_n \ , \quad \phi_i = a_i\phi_{i+1} - b_ic_i\phi_{i+2} \ . \tag{1.3}$$

Notice that θ_k and ϕ_k are the principal minors of A

$$\begin{vmatrix} a_1 & b_1 & & \\ c_1 & \ddots & \ddots & \\ & \ddots & \ddots & b_{k-1} \\ & & c_{k-1} & a_k \end{vmatrix} \quad \text{and} \quad \begin{vmatrix} a_k & b_k & & \\ c_k & \ddots & \ddots & \\ & \ddots & \ddots & b_{n-1} \\ & & c_{n-1} & a_n \end{vmatrix} ,$$

respectively. Observe that $\det A = \theta_n = \phi_1$. Using the classical adjoint process to determine the inverse, we have

$$(A^{-1})_{ij} = \begin{cases} (-1)^{i+j}c_i\cdots c_{j-1}\theta_{i-1}\phi_{j+1}/\theta_n, & \text{if } i \le j \ , \\ (-1)^{i+j}b_j\cdots b_{i-1}\theta_{j-1}\phi_{i+1}/\theta_n, & \text{if } i > j \ , \end{cases} \tag{1.4}$$

where the empty product is equal to 1.

From (1.4) we can derive most of the known formulas for the inverse of a tridiagonal matrix. For example

$$\mu_i = \frac{(-1)^{n+i}}{c_i\cdots c_{n-1}}\,\phi_{i+1} \ .$$

Using second-order linear recurrences, Huang and McColl [16] gave simple formulas for the inverse of general tridiagonal and block tridiagonal matrices. They established the monotone behavior of the recurrences in relation with general properties of the matrix, such as diagonal dominance. In particular, the inverse of a general $n \times n$ tridiagonal matrix could be computed in $n^2 + 7n - 7$ arithmetic operations.

Here we generalize (1.4) for a broader class of matrices: acyclic matrices, i.e., matrices whose graph is a given tree. This subject merits a particular investigation since there are many applications of these more general family of matrices, e.g., to sociology and biology [29, 31, 33] or to chemistry [4].

Notice that a tridiagonal matrix is the weighted adjacency matrix of some directed path. We give a simple numerical example of applying our approach. We also provide an application to sign pattern problems. In the end we show a statistical application. This note gives essentially a theoretical approach to the problem. We do not discuss the stability and the reliability of the formulas.

2. Weighted Digraphs

A graph G consists of a finite set $\mathcal{V}$ whose members are called vertices, and a set $\mathcal{E}$ of 2-subset of $\mathcal{V}$. By a digraph $D = (\mathcal{V}, \mathcal{A})$ we mean the same finite set $\mathcal{V}$, and a subset $\mathcal{A}$ of $\mathcal{V} \times \mathcal{V}$, whose members are called arcs. Note that an arc is an ordered pair (i, j), whereas an edge of a graph is an unordered pair $\{i, j\}$. For background information on graphs and digraphs, we refer the reader to [9]. A forest is a graph without cycles and a tree is a connected forest.

Given an arc $e = (i, j)$ of D, $D \backslash e$ is obtained by deleting e but not the vertices i or j; on other hand $D \backslash i$ is obtained by deleting i and all arcs including i.

Let $A = (a_{ij})$ be an $n \times n$ matrix. The graph of A, $G(A)$, is the pair $(\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \{1, \ldots, n\}$ and $\{i, j\}$ is an edge if and only if and only if $a_{ij} \neq 0$ or $a_{ji} \neq 0$. Analogously the weighted digraph of $A = (a_{ij})$ is such (i, j) is an arc if and only if $a_{ij} \neq 0$, for $i \neq j$. The matrix A can be viewed as a weighted adjacency matrix of digraph $D(A)$ on n vertices, with loops (arcs of the type (i, i)) allowed on the vertices.

A directed path from i_1 to i_r, P_{i_1, i_r}, in the digraph D is a sequence of distinct vertices $(i_1, i_2, \ldots, i_{r-1}, i_r)$ such that each arc $(i_1, i_2), \ldots, (i_{r-1}, i_r)$ is in $\mathcal{A}$. We say that the length of P_{i_1, i_r}, $\ell(P_{i_1, i_r})$, is $r - 1$. If to the path P_{i_1, i_r} we add the arc (i_r, i_1), then we have a cycle (of length r).

3. Inverse of a Tree

The Laplace expansion formula of the determinant of a matrix provides some very interesting connections with graph theory. There are some well known formulas. We will follow the one presented by Maybee and Quirk in [23].

Theorem 1. *Given an $n \times n$ matrix $A = (a_{ij})$ and $i \in \{1, \ldots, n\}$, let us assume that $\{c_1, \ldots, c_m\}$ is the set of all cycles in $D(A) = D$ containing the vertex i, with $\ell_j = \ell(c_j)$. Then*

$$\det A = \sum_{j=1}^{m} (-)^{\ell_j + 1} \det A(D \setminus c_j) \prod_{e \in \mathcal{A}(c_j)} a_e \,. \tag{3.1}$$

Notice that if $D \setminus c_j$ is disconnected, then $\det A(D \setminus c_j)$ is a product of the determinants of the weighted adjacency matrix of each component.

Suppose now that we have an $n \times n$ nonsingular matrix A whose graph is a tree T. In order to determine the inverse of A using the adjoint method, we need to determine each cofactor of A, i.e., substituting in A the row j by row vector equal to zero except the i-entry which is equal to 1, or the column i by column vector equal to zero except the j-entry which is equal to 1, and finally evaluate the determinant. This procedure can be generalized and it is equivalent to eliminate all the arcs starting in the vertex j, except the arc (ji) with weight 1. Since the graph of A is a tree, there will be at most one directed cycle containing j in the new digraph. Suppose that exists one, say c. Then

$$\prod_{e\in\mathcal{A}(c)} a_e = \prod_{e\in\mathcal{A}(P_{ij})} a_e \ .$$

Otherwise, from (3.1), the above product is 0. This leads us to a key result for the inverse of matrix whose graph is a tree.

Theorem 2. *Given an $n \times n$ nonsingular matrix $A = (a_{ij})$ whose graph is a tree, with $D(A) = D$, the inverse $A^{-1} = (\alpha_{ij})$ is given by*

$$\alpha_{ij} = (-)^{\ell_{ij}} \frac{\det A(D \setminus P_{ij})}{\det A} \prod_{e\in\mathcal{A}(P_{ij})} a_e \tag{3.2}$$

if there is a directed path P_{ij}, with ℓ_{ij} the length of P_{ij}, and $\alpha_{ij} = 0$ otherwise.

Notice that the last factor in (3.2) is the product of all weights of the arcs of P_{ij}. We also point out that factor $\det A(D \setminus P_{ij})$ is equal to a product of determinants of tridiagonal matrices. Finally, in the case of $i = j$ we have

$$\alpha_{ii} = \frac{\det A(D \setminus i)}{\det A} \ . \tag{3.3}$$

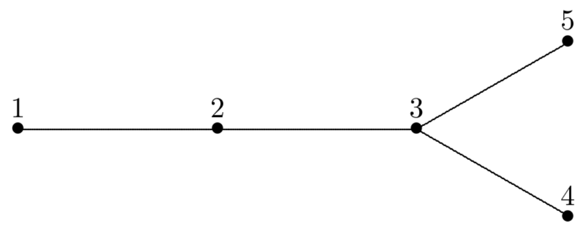
The formulas for the inverse of a tridiagonal matrix (1.1) follow from the Theorem 2. For example, supposing that $i < j$, then $P_{ij} = (i, i+1, \dots, j-1, j)$, and $\prod_{e\in\mathcal{A}(P_{ij})} a_e = c_i \cdots c_{j-1}$ and $\det A(D \setminus P_{ij}) = \theta_{i-1}\phi_{j+1}$, with θ_i and ϕ_j defined as in (1.2) and (1.3), respectively.

4. A Numerical Example

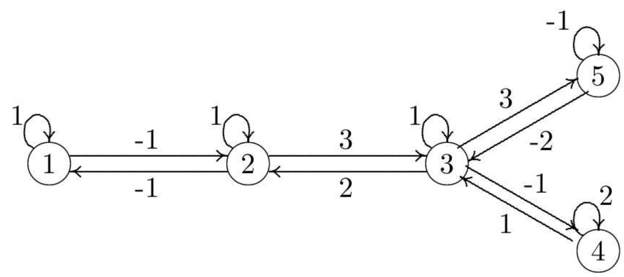
Consider the matrix

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

The graph of A, $G(A)$, is



and the digraph, $D(A)$, is



Using (3.2), we compute, for example, the last row of A^{-1}:

$$\alpha_{51} = \frac{(-1)^3}{12} \cdot 2 \cdot (-2 \cdot 2 \cdot (-1)) = -\frac{8}{12},$$
$$\alpha_{52} = \frac{(-1)^2}{12} \cdot 1 \cdot 2 \cdot (-2 \cdot 2) = -\frac{8}{12},$$
$$\alpha_{53} = \frac{(-1)^1}{12} \cdot \begin{vmatrix} 1 & -1 \\ -1 & 1 \end{vmatrix} \cdot 2 \cdot (-2) = 0,$$
$$\alpha_{54} = \frac{(-1)^2}{12} \cdot \begin{vmatrix} 1 & -1 \\ -1 & 1 \end{vmatrix} \cdot (-2 \cdot (-1)) = 0,$$
$$\alpha_{55} = \frac{1}{12} \begin{vmatrix} -1 & 1 & 0 & 0 \\ -1 & 1 & 3 & 0 \\ 0 & 2 & 1 & -1 \\ 0 & 0 & 1 & 2 \end{vmatrix} = -\frac{12}{12}.$$

Computing the other elements in a similar way, we get

$$A^{-1} = \frac{1}{12} \begin{pmatrix} 21 & 9 & 6 & 3 & 18 \\ 9 & 9 & 6 & 3 & 18 \\ 4 & 4 & 0 & 0 & 0 \\ -2 & -2 & 0 & 6 & 0 \\ -8 & -8 & 0 & 0 & -12 \end{pmatrix}.$$

5. Sign Patterns of the Inverse

In qualitative matrix analysis we study the properties that either require or allow based just upon knowledge of the signs of the entries of a matrix. Qualitative questions on invertibility arise quite often. Here we are interested on the signs of each entry of the inverse, without reference to the magnitudes of the entries of the given matrix. These kind of problems are considered, for example, on the methods of central differences for solving some boundary value problem or on the cubic spline problems (cf. [7]).

We recall that a sign pattern (matrix) is a matrix whose entries are in the set $\{+,-,0\}$.

Following the notation of Section 3, let us assume that $\det A$ and $\det A(D\setminus P)$ are positive, for any directed path P in D starting with a leaf (i.e., a vertex of degree one). It follows from (3.3) that $\alpha_{ii} > 0$, for any $i = 1,\dots,n$. If $(i, i+1)$ is an arc in D, then from (3.2)

$$\alpha_{i,i+1} = -\frac{\det A(D\setminus i, i+1)}{\det A}\, a_{i,i+1}\,,$$

i.e.,

$$\operatorname{sign}\alpha_{i,i+1} = -\operatorname{sign} a_{i,i+1}\ .$$

We can derive other relations for the entries of the inverse. For example, if there is a directed path connecting i and j and (j,k) is an arc, then

$$\operatorname{sign}\alpha_{ik} = -\operatorname{sign}\alpha_{ij}\ \operatorname{sign} a_{jk}\,.$$

Let us consider the matrix

$$A = \begin{pmatrix} 3 & 1 & 0 & 0 & 0 \\ 1 & 4 & 3 & 0 & 0 \\ 0 & 3 & 3 & -1 & 3 \\ 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & -2 & 0 & 1 \end{pmatrix},$$

whose graph is the same Section 3. According to our above considerations, the sign pattern of the inverse of this matrix is

$$\begin{pmatrix} + & - & + & + & - \\ - & + & - & - & + \\ + & - & + & + & - \\ + & - & + & + & - \\ + & - & + & + & + \end{pmatrix}.$$

6. A Statistical Application

Matrix inversion has also many interesting applications in analysis of data. For more details the reader is refer to [14]. For example, overlapping samples occur in many branches of statistics. In [18] Kamps considered in a model of successive pairwise overlap, two parameter estimators for the expectation of underlying random variables. Toeplitz symmetric tridiagonal $n \times n$ matrices of the type

$$\Sigma = \begin{pmatrix} a & b & & & \\ b & a & b & & \\ & b & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ & & & b & a \end{pmatrix}$$

with $a > 2|b| \neq 0$, arise as the covariance matrix of one-dependent random variables $Y_1, \ldots, Y_n$ with same expectation. The least squares estimator

$$\hat{\mu}_{\text{opt}} = \frac{\mathbf{1}^t \Sigma^{-1} Y}{\mathbf{1}^t \Sigma^{-1} \mathbf{1}} \,,$$

where $\mathbf{1} = (1, \ldots, 1)$ and $Y = (Y_1, \ldots, Y_n)^t$, estimates the parameter μ equal to the common expectation of the Y_i's, with variance

$$V(\hat{\mu}_{\text{opt}}) = \frac{1}{\mathbf{1}^t \Sigma^{-1} \mathbf{1}} \,.$$

The estimator $\hat{\mu}_{\text{opt}}$ is the best unbiased estimator based on Y (cf. e.g. [17, 18]). Hence, the sum of all entries of the inverse of Σ, $\mathbf{1}^t \Sigma^{-1} \mathbf{1}$, has an important role in the determination of this estimator and therefore in the computation of the variance $V(\hat{\mu}_{\text{opt}})$. Such model can be generalized in the way that the estimators are based on sample means having an acyclic covariance matrix.

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