Treediagonal Matrices and Their Inverses

D. J. Klein
Department of Marine Sciences
Texas A & M University at Galveston
Galveston, Texas 77553

Submitted by Richard A. Brualdi

ABSTRACT

A generalization of tridiagonal matrices is considered, namely treediagonal matrices, which have nonzero off-diagonal elements only in positions where the adjacency matrix of a tree has nonzero elements. Some properties of treediagonal matrices are given, and their inverses are characterized and shown to have an interesting structure.

1. TREEDIAGONAL MATRICES

We recall a few elementary graph-theoretical terms (see, e.g., [1]). Let Γ denote a graph with vertex set $\mathcal{V}=\{1,2,\dots,N\}$ and edge set $\mathcal{E}$, which consists of (unordered) pairs of vertices. A subgraph of Γ is a graph with vertex and edge sets which are subsets of $\mathcal{V}$ and $\mathcal{E}$. A subgraph is a spanning subgraph of Γ if its vertex set is $\mathcal{V}$ also. If Γ is connected and acyclic, then Γ is said to be a tree. Let v_i denote the valence (or degree) of a vertex i. Vertices of valence 1 are termed end vertices, and those of valence $\geqslant 2$ are termed interior. The neighborhood of $i\in\mathcal{V}$ is the set $N(i)=\{j\in\mathcal{V};\ \{i,j\}\in\mathcal{E}\}$.

Throughout this paper we assume Γ is a tree. Further, we consider N-by-N matrices whose rows, and columns, are labeled by the vertices of $\mathcal{V}$. We define a matrix A to be treediagonal (or more explicitly Γ-treediagonal) if the matrix elements A_{ij} of A are such that $A_{ij}=0$ for $i\neq j$ and $\{i,j\}\notin\mathcal{E}$. Such matrices and the associated inversion algorithms have already been studied [2–4]. Clearly, if Γ is a linear path, then Γ is equivalent via a simultaneous permutation of row and column indices to a tridiagonal matrix; indeed, A is explicitly tridiagonal if $\mathcal{E}=\{\{i,i+1\};\ i=1 \text{ to } N-1\}$.

Treediagonal matrices have a number of properties and characteristics reminiscent of the more special tridiagonal matrices. Indeed, most (but not all) of the results we obtain are already known [5, 6] for the tridiagonal case. In this section our results involve especially simple extensions of properties of

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tridiagonal matrices and are presented without detailed proof. The main results come in Sections 3 and 4 and are extensions of recent work by Barrett [6].

Since an N-vertex tree has $N-1$ edges (as is readily seen by an induction argument), one sees

PROPOSITION 1. *Γ-treediagonal matrices can have up to but no more than $2(N-1)$ nonzero off-diagonal elements.*

If $\{i_1, i_2, \dots, i_n\} \in \mathcal{V}$, then let $\Gamma_{(i_1,\dots,i_n)}$ denote the graph obtained from Γ on deleting the vertices $i_1,\dots,i_n$ and their incident edges; further let $\Delta_{(i_1,\dots,i_n)}$ denote the determinant obtained from A on deleting rows and columns $i_1,\dots,i_n$, and let Δ denote $\det A$. Now using the familiar expansion of a determinant in minors (first along row i and then for the second term along column i), one obtains

PROPOSITION 2. *If A is a treediagonal matrix with i an end vertex and j its neighbor, then*

$$\Delta = A_{ii}\Delta_{(i)} - A_{ij}A_{ji}\Delta_{(i,j)}$$

Here $\Delta_{(i)}$ and $\Delta_{(i,j)}$ are determinants for $\Gamma_{(i)}$- and $\Gamma_{(i,j)}$-treediagonal matrices, so that this proposition could be iterated. Indeed, it could be used to evaluate sequences of determinants $\Delta_{(i_1,i_2,\dots,i_m)}$, $m=1$ to $N-1$, with $i_1, i_2, \dots, i_{N-1}$ each an end vertex after removing preceding vertices. Then just as in the well-known [3] Givens and Householder "matrix diagonalization" algorithms, the sign-change counting method for localizing eigenvalues of tridiagonal Hermitian matrices may be applied to Hermitian treediagonal matrices. Proposition 2 also leads to

PROPOSITION 3. *If A is a treediagonal matrix, then its determinant is given as*

$$\Delta = \sum_{\gamma \subset \Gamma} (-1)^{|\mathfrak{E}^{\gamma}|} \prod_{\{i,j\}\in \mathfrak{E}^{\gamma}} A_{ij}A_{ji} \prod_{\{k:\, v_k^{\gamma}=0\}} A_{kk},$$

where the sum is over all spanning subgraphs γ of Γ such that all vertices have valence 0 or 1. Also $\mathfrak{E}^{\gamma}$ is the edge set of γ, $|\mathfrak{E}^{\gamma}|$ the number of edges in $\mathfrak{E}^{\gamma}$, and v_k^{γ} the valence of the kth vertex in γ. (If either of the products in this equation is vacuous, the product is taken to be unity.)

Also a ready consequence of Propositions 2 and 3 is

PROPOSITION 4. *If A is a treediagonal matrix, then its permanent is given as*

$$\operatorname{per} A = \sum_{\gamma \subset \Gamma} \prod_{\{i,j\} \in \mathcal{E}^{\gamma}} A_{ij} A_{ji} \prod_{\{k: v_k^{\gamma} = 0\}} A_{kk} = \det \hat{A},$$

where the sum is as in Proposition 3 *and* $\hat{A}$ *is a matrix with*

$$\hat{A}_{ij} = \begin{cases} +A_{ij}, & i \geq j, \\ -A_{ij}, & i < j. \end{cases}$$

A finite constructive method for transforming a general square matrix to a given general Γ-treediagonal form does not yet seem to be known.

2. INVERSES OF TREEDIAGONAL MATRICES

For a given tree Γ let $[i, j]$ denote the (unique) path from vertex i to j; that is,

$$[i_1, i_n] = (i_1, i_2, \ldots, i_n), \qquad \text{where} \quad \{i_a, i_{a+1}\} \in \mathcal{E}, \quad a = 1 \text{ to } n-1.$$

We say $k \in [i_1, i_n]$ if k is one of these i_a. For a Γ-treediagonal matrix A with $[i_1, i_n]$ as above, define

$$p[i_1, i_n] = \begin{cases} 1, & n = 1, \\ \prod_{a=1}^{n-1} A_{i_a i_{a+1}}, & n \geq 2. \end{cases}$$

Further let $|[i_1, i_n]| = n - 1$ denote the length of $[i_1, i_n]$.

THEOREM 1. *If A is a nonsingular treediagonal matrix, then*

$$(A^{-1})_{ij} = (-1)^{|[i,j]|} p[i,j] \Delta_{([i,j])} / \Delta.$$

Further, if $\Gamma_{([i,j])}$ *is disconnected, then* $\Delta_{([i,j])}$ *factors, with each factor being the determinant of the matrix for the associated component of* $\Gamma_{([i,j])}$.

Proof. We use the standard formula

$$(A^{-1})_{ij}=\frac{(-1)^{i+j}}{\Delta}\det A_{(j|i)},$$

where $A_{(j|i)}$ denotes the matrix obtained on deleting the jth row and ith column of A. Consider the matrix A' which is the same as A except that its (j,i)th element is replaced by $A'_{ji}=1$. Now

$$\det A'=\sum_{\pi}(-1)^{\pi}\prod_{k=1}^{N}A'_{k\pi(k)}$$

where the sum is over all $N!$ permutations π, $(-1)^{\pi}$ is the parity of π, and $\pi(k)$ is the image of k under π. Then since the determinant function involves sums over products with exactly one element from each row and column, we see that $(-1)^{i+j}\det A_{(j|i)}$ is simply the portion of the π-sum above for which $\pi(j)=i$. For a π giving a nonzero contribution, each cycle in π must correspond to a cycle of nonzero elements in the graph Γ' of A'. Here Γ' includes $\{i,j\}$ in its edge set, but is otherwise the same as Γ. For the π giving a nonzero contribution we then seek a path in Γ from i to j, and π must involve a cycle cyclically permuting the vertices of this path $[i,j]$. Since the path length is $|[i,j]|$, the parity of this cycle is $(-1)^{|[i,j]|}$. Hence

$$(-1)^{i+j}\det A_{(j|i)}=(-1)^{|[i,j]|}p[i,j]\sum_{\pi'}(-1)^{\pi'}\prod_{k\notin[i,j]}A_{k\pi'(k)},$$

where π' is restricted to permutations of vertices other than those in $[i,j]$. Since this π'-sum yields just $\det A_{([i,j])}$, the first part of the theorem is established. The second part of the theorem is seen on noting that the disjoint components of $\Gamma_{([i,j])}$ correspond to disconnected blocks of the matrix obtained from A on deleting the rows and columns of $[i,j]$. ■

THEOREM 2. *Let A be a treediagonal matrix with $\Delta_{(\mathcal{S})}\neq 0$, for all $\mathcal{S}\subseteq\mathcal{V}$ associated with a connected subtree of Γ. Define generalized continued fractions via the recurrence relations*

$$f_i=A_{ii}-\sum_{j\in N(i)}\frac{A_{ij}A_{ji}}{f_{(i)j}}$$

$$f_{(i_1,\ldots,i_m)i}=A_{ii}-\sum_{j\in N(i),\,j\neq i_m}\frac{A_{ij}A_{ji}}{f_{(i_1,\ldots,i_m,i)j}},\qquad m\geq 1,$$

where $[i_1, i_m]$ is a path in Γ, $\{i_m, i\} \in \mathcal{E}$, and where termination points are reached whenever the j-sum becomes vacuous. Then A^{-1} is given as

$$(A^{-1})_{ii} = 1/f_i,$$

$$(A^{-1})_{i_1 i_m} = (-1)^{m-1} p[i_1, i_m] \frac{1}{f_{i_1}} \prod_{a=1}^{m-1} \frac{1}{f_{(i_1, \ldots, i_a) i_{a+1}}}, \qquad m \geq 2.$$

This may be proven using Theorem 1 and noting that the ratio $\Delta/\Delta_{(i)}$ in place of f_i and the ratios $\Delta_{(i_1, \ldots, i_m)}/\Delta_{(i_1, \ldots, i_m, i)}$ in place of $f_{(i_1, \ldots, i_m)i}$ satisfy the same recurrence relations, as may be seen by expanding the numerators along row i. There is another proof [3] which follows earlier work [7] relating tridiagonal matrices, their inverses, and ordinary continued fractions. Further analogies between the generalized continued fractions of Theorem 2 and ordinary ones seem to be little developed.

3. TREEANGLE PROPERTY FOR MATRICES

For a given tree Γ an N-by-N matrix R satisfies the treeangle (or more explicitly Γ-treeangle) property if for every $i, j, k \in \mathcal{V}$ with $k \in [i, j]$,

$$R_{ij} R_{kk} = R_{ik} R_{kj}.$$

If Γ is a path, this treeangle property, along with the requirement that $R_{kk} \neq 0$ for interior vertices, yields Barrett's [2] triangle property.

If R satisfies the treeangle property and $R_{ii} \neq 0$ for interior vertices, repetitive use of the treeangle property gives

$$R_{i_1 i_n} = R_{i_1 i_2} \prod_{a=2}^{n-1} \frac{R_{i_a i_{a+1}}}{R_{i_a i_a}}, \qquad [i_1, i_n] = (i_1, i_2, \ldots, i_n), \quad n \geq 3.$$

Note that $R_{i_1 i_n}$ has a visual interpretation as a ratio of the product of the elements of R labeled by the (directed) edges of the path $[i_1, i_n]$ to the product of the elements of R labeled by the interior vertices of the path. Hence all the elements of R are determined from a knowledge of the diagonal elements and those $2(N-1)$ off-diagonal elements R_{ij} for which $\{i, j\} \in \mathcal{E}$.

In the following we utilize the definition

$$d_{ij} = R_{ii} R_{jj} - R_{ij} R_{ji}.$$

Further we let I denote the N-by-N identity matrix, ∇ denote the determinant of $R-xI$, and for $n=1,\ldots,N-1$, $\nabla_{(i_1,\ldots,i_n)}$ denote the determinant of the matrix obtained from $R-xI$ by deleting rows and columns $i_1,\ldots,i_n$.

THEOREM 3. *If R satisfies the treeangle property and if i is an end vertex with $R_{ij}\neq 0$ for the vertex j adjacent to i, then*

$$\nabla=\left\{\frac{d_{ij}}{R_{ij}}-x-\frac{R_{ij}R_{ji}}{R_{ij}^2}x\right\}\nabla_{(i)}-\frac{R_{ij}R_{ji}}{R_{ij}^2}x^2\nabla_{(i,j)}. \tag{3.1}$$

Proof. We let $R'=R-xI$ and expand by minors along the ith row:

$$\nabla=(R_{ii}-x)\nabla_{(i)}+\sum_{k\neq i}(-1)^{i+k}R_{ik}\det R'_{(i|k)}.$$

Now we use the treeangle property to replace R_{ik} by $R_{ij}R_{jk}/R_{jj}$, and then rearrange the equation to obtain

$$\nabla=(R_{ii}-x)\nabla_{(i)}+\frac{R_{ij}}{R_{jj}}\left\{-R_{ij}\det R'_{(i|i)}+(-1)^{i+j}x\det R'_{(i|j)}\right.$$

$$\left.+\sum_k(-1)^{i+k}R'_{jk}\det R'_{(i|k)}\right\}. \tag{3.2}$$

Here the last k-sum is just the determinant of the matrix with row i replaced by row j, and hence gives zero. Next we expand

$$\det R'_{(i|j)}=\sum_{l\neq i}(-1)^{i+l+\delta}R_{li}\det R'_{(il|ij)},$$

where $R'_{(il|ij)}$ denotes the matrix obtained from R' on deleting rows i,l and columns i,j. Further, here $\delta=0$ if $l<i<j$ or $l>i>j$, and $\delta=1$ otherwise. Now we replace R_{li} by $R_{lj}R_{ji}/R_{jj}$ and rearrange the equation to obtain

$$\det R'_{(i|j)}=\frac{R_{ji}}{R_{jj}}\left\{(-1)^{i+j+1}x\det R'_{(ij|ij)}+\sum_{l\neq i}(-1)^{i+l+\delta}R'_{lj}\det R'_{(il|ij)}\right\}.$$

Expanding $\det R'_{(i|i)}$ by minors along the jth column, one sees that the last

l-sum is just $(-1)^{i+j+1}\det R'_{(i|i)}$. Substituting back into Equation (3.2) yields Equation (3.1).

Remarks similar to those following Proposition 2 apply. Further, if one specializes Theorem 3 to $x=0$ and applies it in an iterative manner one obtains

COROLLARY. *If R satisfies the treeangle property with $R_{kk}\neq 0$ for interior vertices $k\in\mathcal{V}$, then*

$$\det R=\prod_{\{i,j\}\in\mathcal{E}} d_{ij}\prod_{k=1}^{n} R_{kk}^{1-v_k},$$

where R_{kk}^{0} is understood to always equal 1.

This result is given by Barrett [6] for the special case of the triangle property.

4. TREEDIAGONALITY AND THE TREEANGLE PROPERTY

The interrelation between treediagonal and treeangle properties found in this section are again extensions of Barrett's work [6].

THEOREM 4. *If a nonsingular matrix R satisfies the treeangle property with $R_{jj}\neq 0$ for interior vertices $j\in\mathcal{V}$, then the treediagonal matrix A with elements*

$$A_{ik}=\begin{cases} -R_{ik}/d_{ik}, & \{i,k\}\in\mathcal{E},\\ R_{jj}/d_{ij}, & i=k,\quad v_i=1,\quad \{i,j\}\in\mathcal{E},\\ \left(1+\displaystyle\sum_{j\in N(i)}\frac{R_{ij}R_{ji}}{d_{ij}}\right)\dfrac{1}{R_{ii}}, & i=k,\quad v_i\geqslant 2,\\ 0 & \text{otherwise}\end{cases}$$

is the inverse to R.

Proof. First, the corollary to Theorem 3 implies that in order for R to be nonsingular all d_{ij} for $\{i,j\}\in\mathcal{E}$ must be nonzero. Then the matrix is well defined, and we proceed to show it is the inverse of R. For $v_i=1$ and

$\{i,j\}\in\mathcal{E}$,

$$1+\frac{R_{ij}R_{ji}}{d_{ij}}=\frac{R_{ii}R_{jj}}{d_{ij}}=R_{ii}A_{ii},$$

so that for all i

$$R_{ii}A_{ii}=1+\sum_{j\in N(i)}\frac{R_{ij}R_{ji}}{d_{ij}}.$$

It follows that

$$(RA)_{ii}=R_{ii}A_{ii}+\sum_{j\in N(i)}R_{ij}\left(-\frac{R_{ji}}{d_{ij}}\right)=R_{ii}A_{ii}-(R_{ii}A_{ii}-1)=1.$$

Next if $i\neq k$, and $j\in[i,k]$ is such that $\{j,k\}\in\mathcal{E}$, then

$$(RA)_{ik}=R_{ik}A_{kk}+R_{ij}\left(-\frac{R_{jk}}{d_{jk}}\right)+\sum_{l\in N(k),\,l\neq j}R_{il}\left(-\frac{R_{lk}}{d_{lk}}\right).$$

If the l-sum here is vacuous, then $v_k=1$ and

$$(RA)_{ik}=R_{ik}\frac{R_{jj}}{d_{jk}}-R_{ij}\frac{R_{jk}}{d_{jk}}=0,$$

whereas if the l-sum is not vacuous, then $R_{kk}\neq 0$ and

$$\begin{aligned}(RA)_{ik}&=R_{ik}A_{kk}-R_{ik}\frac{R_{jj}}{d_{jk}}-\sum_{l\in N(k),\,l\neq j}\frac{R_{ik}R_{kl}}{R_{kk}}\frac{R_{lk}}{d_{lk}}\\&=R_{ik}\left\{A_{kk}-\frac{1}{R_{kk}}\left(1+\sum_{l\in N(k)}\frac{R_{kl}R_{lk}}{d_{lk}}\right)\right\}\\&=0.\end{aligned}$$

Hence RA is the identity matrix and the theorem is established. ■

THEOREM 5. *If A is a nonsingular treediagonal matrix, then its inverse satisfies the treeangle property.*

Proof. We utilize the formula and results of Theorem 1 for $(A^{-1})_{ij}$. Now $\Delta_{([i,j])}$ is the product of the determinants associated with the separate disconnected components of $\Gamma_{([i,j])}$. Thus for $j \in [i, k]$

$$\Delta_{([i,j])}\Delta_{([j,k])} = \Delta_{([i,k])}\Delta_{(j)},$$

since the different disconnected components of the various graphs on the left- and right-hand sides of this equation are the same. Further one easily verifies

$$p[i,j]p[j,k] = p[i,k]p[j,j]$$

and a similar relation involving parities. Hence using the formula of Theorem 1, we obtain

$$(A^{-1})_{ij}(A^{-1})_{jk} = (A^{-1})_{ik}(A^{-1})_{jj},$$

the desired result. ∎

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