On some matrices related to a tree with attached graphs

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Abstract

A tree with attached graphs is a tree, together with graphs defined on its partite sets. In an earlier paper, we introduced the notion of the incidence matrix $Q$ and the Laplacian $L = QQ'$ for a tree with attached graphs. Here we consider the case when the attached graphs are trees. We obtain formulas for the Moore-Penrose inverse of $Q$ and for the inverse of $K = Q'Q$, thereby extending some work in the literature, including a formula by Merris proved in the case of a tree. The case when the attached graphs are paths is related to the basic feasible solutions in a transportation problem.

Key words and phrases: tree, incidence matrix, Moore-Penrose inverse, transportation problem, edge Laplacian matrix

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1 Introduction

Minors of matrices associated with a graph have been an area of considerable interest, starting with the celebrated Matrix Tree Theorem of Kirchhoff, which asserts that any cofactor of the Laplacian matrix equals the number of spanning trees in the graph. Several papers have been devoted to the theme of Matrix Tree type theorems; see [3, 4, 8, 12] for more information and further references. Combinatorial interpretation of minors is closely related to interpreting the inverse, or a generalized inverse, of the matrix. As an example, the Moore-Penrose inverse of the Laplacian matrix has been investigated in [1, 10].

In a recent paper [2] we introduced the concept of a tree with attached graphs, which is simply a tree with graphs defined on its partite sets. The notions of incidence matrix, Laplacian and distance matrix were defined for a tree with attached graphs. In the present paper we consider the case when the attached graphs are trees. Formulas are obtained for the Moore-Penrose inverse of the incidence matrix $Q$ and for the inverse of $K = Q'Q$. When one of the partite sets has only one vertex, these results reduce to known formulae [1, 11] for the case of a tree. Another special case of a tree with attached graphs that is of interest is when the attached graphs are paths. It is related to basic feasible solutions in a transportation problem. This is illustrated in Section 5.

2 Preliminaries

We consider simple graphs, that is, graphs that have no loops or parallel edges. The vertex set and the edge set of the graph $G$ are denoted by $V(G)$ and $E(G)$ respectively. The transpose of a matrix $A$ is denoted $A'$. If $G$ is a directed graph with $n$ vertices and $m$ edges, then its incidence matrix $Q$ is the $n \times m$ matrix defined as follows. The rows and the columns of $Q$ are indexed by $V(G)$ and $E(G)$ respectively. If $i \in V(G)$ and $j \in E(G)$, then the $(i, j)$-entry of $Q$ is 0 if vertex $i$ and edge $j$ are not incident and otherwise it is 1 or $-1$ according
as \( j \) originates or terminates at \( i \) respectively. The Laplacian matrix \( L \) of \( G \) is defined as \( L = QQ' \). The Laplacian does not depend on the orientation and thus is defined for an undirected graph. We assume familiarity with basic properties of the incidence matrix and the Laplacian; see, for example, [5, 12, 15]. The vector of appropriate size with each entry equal to one will be denoted by \( 1 \).

We now introduce some more definitions. If \( A \) is an \( n \times m \) matrix, then an \( m \times n \) matrix \( H \) is called a generalized inverse (or a \( g \)-inverse) of \( A \) if \( AHA = A \). The Moore-Penrose inverse of \( A \) is an \( m \times n \) matrix \( H \) satisfying the equations \( AHA = A, HAH = H, (AH)' = AH \) and \( (HA)' = HA \). It is well-known that the Moore-Penrose inverse exists and is unique. We denote the Moore-Penrose inverse of \( A \) by \( A^+ \). For background material on generalized inverses, see [6, 7].

The following notation will be used in the rest of the paper. Let \( T \) be a tree with \( |V(T)| = n + 1 \). We assume \( n \geq 2 \). Let \( X_1 \) and \( X_2 \) be partite sets of \( T \) with \( |X_1| = p_1, |X_2| = p_2, p_1 + p_2 = n + 1 \). Let \( G_i \) be a connected, directed graph with \( V(G_i) = X_i \) and \( |E(G_i)| = m_i, i = 1, 2 \). We assume that the edges of \( T \) are directed as well and, for convenience, we take them to be oriented from \( X_1 \) to \( X_2 \). We think of the graph \( T \cup G_1 \cup G_2 \) as a tree \( (T) \) with attached graphs \( (G_1, G_2) \).

Let \( A \) be the \((n + 1) \times n \) incidence matrix of \( T \) and let \( B_i \) be the \( p_i \times m_i \) incidence matrix of \( G_i, i = 1, 2 \). We set

\[
B = \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}.
\] (1)

We remark that if \( p_2 = 1 \), then \( B_2 \) is vacuous and the last row of \( B \) consists of all zeros. The columns of \( A \) are linearly independent. Thus there is a unique \( n \times (m_1 + m_2) \) matrix \( Q \) satisfying \( AQ = B \). We call \( Q \), the incidence matrix, and \( L = QQ' \), the Laplacian, of \( T \cup G_1 \cup G_2 \). The rows and the columns of \( Q \) are indexed by \( E(T) \) and \( E(G_1) \cup E(G_2) \) respectively. The incidence vector of an edge of \( G_1 \cup G_2 \) is a unique linear combination, with coefficients 0, ±1, of the
columns of $A$, and the corresponding column of $Q$ merely lists the coefficients in such a linear combination. In particular, since the edges of $T$ are all oriented from $X_1$ to $X_2$, the sum of the entries in every column of $Q$ is zero. We also note some elementary properties of $L$. Clearly $L$ is $n \times n$, symmetric, positive semidefinite, and has rank $n - 1$. The entries of $L$ are integers, but in contrast to the Laplacian of a graph, it does not necessarily have nonpositive off-diagonal entries.

In this paper we consider the case when $G_1$ and $G_2$ are trees. Thus let $T_1$ and $T_2$ be directed trees on $X_1$ and $X_2$ respectively, and consider the tree with attached graphs, $T \cup T_1 \cup T_2$. The orders of the matrices $A$, $B$ and $Q$ are, respectively, $(n + 1) \times n$, $(n + 1) \times (n - 1)$ and $n \times (n - 1)$. The rows and columns of $Q$ are indexed by $E(T)$ and $E(T_1 \cup T_2)$ respectively. As observed in [2], $Q$ is totally unimodular, and in particular, all its entries are $0$ or $\pm 1$.

3 Moore-Penrose inverse of $Q$

Let $\tilde{T}$ be a directed tree and let $e \in E(\tilde{T})$. Clearly, $\tilde{T} \setminus e$ is a forest with two components. The component of $\tilde{T} \setminus e$ that contains the head (respectively, tail) of $e$ will be called the head-tree (respectively, tail-tree) of $\tilde{T} \setminus e$. We denote the head-tree of $\tilde{T} \setminus e$ by $H(\tilde{T} \setminus e)$ and the tail-tree of $\tilde{T} \setminus e$ by $T(\tilde{T} \setminus e)$.

We continue to work with the notation introduced in the previous section.

**Lemma 1** Define the $(n - 1) \times n$ matrix $G$ as follows. The rows and the columns of $G$ are indexed by $E(T_1 \cup T_2)$ and $E(T)$ respectively. If $e \in E(T_1)$ and $f \in E(T)$, then the $(e, f)$-element of $G$ is $1$ if $f$ is incident to $T(T_1 \setminus e)$ and $0$ otherwise. If $e \in E(T_2)$ and $f \in E(T)$, then the $(e, f)$-element of $G$ is $1$ if $f$ is incident to $H(T_2 \setminus e)$ and $0$ otherwise. Then $G$ is a left-inverse of $Q$.

**Proof:** Let $e \in E(T_1 \cup T_2)$ and consider the $(e, e)$-element of $GQ$. The $e$-th column of $Q$ is the incidence vector of the directed path from the tail of $e$ to the head of $e$. Thus the inner product of the $e$-th column of $Q$ and the $e$-th
row of $G$ is 1. Similarly, if $e, f \in E(T_1 \cup T_2), e \neq f$, then it can be seen that the $(e, f)$-element of $GQ$ is zero. Thus $GQ = I$ and the proof is complete. ■

In the next result we present a formula for $Q^+$.

**Theorem 2** The rows and the columns of $Q^+$ are indexed by $E(T_1 \cup T_2)$ and $E(T)$ respectively. Let $e \in E(T_1 \cup T_2)$ and $f \in E(T)$.

Case (i): $e \in E(T_1)$. If $f$ is incident to a vertex in $T(T_1 \setminus e)$, then the $(e, f)$-entry of $Q^+$ equals $\frac{1}{n}$ times the number edges of $T$ incident to $H(T_1 \setminus e)$. If $f$ is incident to a vertex in $H(T_1 \setminus e)$, then the $(e, f)$-entry of $Q^+$ equals $-\frac{1}{n}$ times the number of edges of $T$ incident to $T(T_1 \setminus e)$.

Case (ii): $e \in E(T_2)$. If $f$ is incident to a vertex in $H(T_2 \setminus e)$, then the $(e, f)$-entry of $Q^+$ equals $\frac{1}{n}$ times the number of edges of $T$ incident to $T(T_2 \setminus e)$. If $f$ is incident to a vertex in $T(T_2 \setminus e)$, then the $(e, f)$-entry of $Q^+$ equals $-\frac{1}{n}$ times the number of edges of $T$ incident to $H(T_2 \setminus e)$.

**Proof:** The set of g-inverses of $Q$ is given by (see [14], p.25) matrices of the form

$$G + X - GQXGQ$$

where $G$ is the g-inverse given in Lemma 1 and $X$ is arbitrary. As noted in Lemma 1, $GQ = I$. Furthermore, $I - QG$ is the projection matrix on the null-space of $Q'$. Since the null-space of $Q'$ is one-dimensional and is spanned by the vector of all ones, $I - QG$ equals a scalar multiple of the matrix of all ones.

Thus, in view of (2), the class of g-inverses of $Q$ is seen to be matrices of the form

$$G + \begin{bmatrix}
\alpha_1 \\
\vdots \\
\alpha_{n-1}
\end{bmatrix}
\begin{bmatrix}
1 & \cdots & 1
\end{bmatrix},$$

where $\alpha_1, \ldots, \alpha_{n-1}$ are arbitrary.
Suppose
\[ Q^+ = G + \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_{n-1} \end{bmatrix} \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}. \] (3)

Since \( Q^+ 1 = 0 \), then from the preceding equation,
\[ \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_{n-1} \end{bmatrix} = -\frac{1}{n} G 1. \] (4)

The result follows from Lemma 1 and the formulae (3), (4).

We remark that when \( T_2 \) has only one vertex, Theorem 2 specializes to the formula for the Moore-Penrose inverse of the incidence matrix of a tree given in [1]. This will be elaborated in Section 5.

4 Inverse of \( K = Q'Q \).

When \( Q \) is the incidence matrix of a tree, the matrix \( K = Q'Q \) has been termed the edge Laplacian by Merris [11], who obtains a formula for the inverse of \( K \). Later, Moon [13] presented another proof of the same formula. In this section we generalize the formula to the present setup.

We continue to follow the notation introduced in Sections 2,3. Let \( K = Q'Q \). Clearly, \( K \) is of order \((n-1) \times (n-1)\) with rank \( K = \text{rank } Q = n-1 \). Since the minors of \( Q \) of order \((n-1) \times (n-1)\) are all equal to \( \pm 1 \), a simple application of the Cauchy-Binet formula shows that \( \det K = n \). We now present a formula for \( K^{-1} \).

**Theorem 3** The rows and the columns of \( K^{-1} \) are indexed by \( E(T_1 \cup T_2) \). Let \( e, f \in E(T_1 \cup T_2) \).

Case (i): \( e, f \in E(T_1) \) and they are similarly oriented, i.e., the unique path in \( T_1 \) from \( e \) to \( f \) goes from the head of \( e \) to the tail of \( f \), or vice versa. Let \( a \)
be the number edges of $T$ incident to both $T(T_1 \setminus e)$ and $T(T_1 \setminus f)$, and let $c$ be the number of edges of $T$ incident to both $\mathcal{H}(T_1 \setminus e)$ and $\mathcal{H}(T_1 \setminus f)$. Then the $(e, f)$-element of $K^{-1}$ is given by $\frac{ac}{n}$.

Case (ii): $e, f \in E(T_1)$ and they are oppositely oriented, i.e., the unique path in $T_1$ from $e$ to $f$ goes from the head of $e$ to the head of $f$, or from the tail of $e$ to the tail of $f$. Let $a, c$ be as defined in Case (i). Then the $(e, f)$-element of $K^{-1}$ is given by $-\frac{ac}{n}$.

If $e, f \in E(T_2)$, then two cases arise, depending on whether $e$ and $f$ are similarly or oppositely oriented. These are similar to Cases (i) and (ii).

Case (iii): $e \in E(T_1), f \in E(T_2)$. Let $a$ be the number of edges of $T$ incident to both $T(T_1 \setminus e)$ and $\mathcal{H}(T_2 \setminus f)$, let $b$ be the number of edges of $T$ incident to both $T(T_1 \setminus e)$ and $T(T_2 \setminus f)$, let $c$ be the number of edges of $T$ incident to both $\mathcal{H}(T_1 \setminus e)$ and $\mathcal{H}(T_2 \setminus f)$, and let $d$ be the number of edges of $T$ incident to both $\mathcal{H}(T_1 \setminus e)$ and $T(T_2 \setminus f)$. Then the $(e, f)$-element of $K^{-1}$ is given by $\frac{ad-bc}{n}$.

Proof: Since $K^{-1} = Q^+(Q^+)'$, the $(e, f)$-element of $K^{-1}$ is given by

$$
\sum_{j \in E(T)} q^+_{ej} q^+_f j.
$$

(5)

First consider Case (i). Let $a$ and $c$ be as defined in Case (i) and let $b$ be the number of edges of $T$ incident to both $\mathcal{H}(T_1 \setminus e)$ and $T(T_1 \setminus f)$.

If $j \in E(T)$ is incident to both $T(T_1 \setminus e)$ and $T(T_1 \setminus f)$, then, using Theorem 2, $q^+_e q^+_j = \frac{b+c}{n} \cdot \frac{c}{n}$. If $j \in E(T)$ is incident to both $\mathcal{H}(T_1 \setminus e)$ and $T(T_1 \setminus f)$, then $q^+_e q^+_j = -\frac{a}{n} \cdot \frac{c}{n}$. Finally, if $j \in E(T)$ is incident to both $\mathcal{H}(T_1 \setminus e)$ and $\mathcal{H}(T_1 \setminus f)$, then $q^+_e q^+_j = \frac{a}{n} \cdot \frac{a+b}{n}$. Substituting in (5) we see that

$$
\sum_{j \in E(T)} q^+_e q^+_j = \frac{1}{n^2} \{(b+c)ca - acb + a(a+b)c\}
$$

$$
= \frac{1}{n^2} \{abc + ac^2 - abc + a^2c + abc\}
$$

$$
= \frac{1}{n^2} ac(a + b + c)
$$

$$
= \frac{ac}{n}
$$

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and the proof is complete in this case.

The proof is similar for Case (ii). Now suppose Case (iii) holds and let \( a, b, c \) and \( d \) be as defined in Case (iii). If \( j \in E(T) \) is incident to both \( T(T_1 \setminus e) \) and \( H(T_2 \setminus f) \), then, using Theorem 2, \( n^2 q^+_{e_j} q^+_{f_j} = a(c + d)(b + d) \). If \( j \in E(T) \) is incident to both \( T(T_1 \setminus e) \) and \( T(T_2 \setminus f) \), then, \( n^2 q^+_{e_j} q^+_{f_j} = -b(c + d)(a + c) \). If \( j \in E(T) \) is incident to both \( H(T_1 \setminus e) \) and \( H(T_2 \setminus f) \), then, \( n^2 q^+_{e_j} q^+_{f_j} = -c(a + b)(b + d) \). If \( j \in E(T) \) is incident to both \( H(T_1 \setminus e) \) and \( T(T_2 \setminus f) \), then, \( n^2 q^+_{e_j} q^+_{f_j} = d(a + b)(a + c) \).

Substituting in (5) we see that

\[
\sum_{j \in E(T)} q^+_{e_j} q^+_{f_j} = \frac{1}{n^2} \left\{ (c + d)(ab + ad - ab - bc) + (a + b)(ad + cd - bc - cd) \right\}
\]

\[
= \frac{1}{n^2} \left\{ (c + d)(ad - bc) + (a + b)(ad - bc) \right\}
\]

\[
= \frac{1}{n^2} (ad - bc)(a + b + c + d)
\]

\[
= \frac{ad - bc}{n}
\]

and the proof is complete.

5 Special cases

Two special cases of the general setup considered in Sections 2–4 are of interest. The first is the case when \( T \) is a star. Thus suppose \( |X_2| = 1 \). As remarked earlier, the matrix \( B_2 \) in (1) is vacuous in this case. However, \( B \) continues to have the last row of all zeros. The \( n \times n \) submatrix of \( A \) formed by the first \( n \) rows is the identity matrix of order \( n \). A left-inverse of \( A \) is given by the identity matrix of order \( n \) augmented by a column of zeros. Thus \( Q \) is seen to equal \( B_1 \). There is a one-to-one correspondence between the edges of \( T \) and \( X_1 = V(G_1) \). Thus the results obtained in this paper specialize to results about the incidence matrix of \( G_1 \). (Of course, in the present paper \( G_1 \) is a tree.)

The second special case of interest arises when \( G_1 \) and \( G_2 \) are paths. We
first introduce some notation. Consider a transportation problem with a set of sources $\mathcal{S}$, with $|\mathcal{S}| = p$, and a set of destinations, $\mathcal{D}$, with $|\mathcal{D}| = q$. To any feasible solution of the problem we may associate a bipartite graph. The partite sets of the graph are $\mathcal{S}$ and $\mathcal{D}$. We assume that the elements of $\mathcal{S}$ and $\mathcal{D}$ are numbered $1, \ldots, p$ and $1, \ldots, q$ respectively. If $i \in \mathcal{S}$ and $j \in \mathcal{D}$, then there is an edge from $i$ to $j$ if and only if a positive quantity is shipped from source $i$ to destination $j$. It is well-known (see, for example, [9]) that such a bipartite graph is a tree if and only if the corresponding feasible solution is a basic feasible solution. From now onwards we assume that $T$ is a tree corresponding to a basic feasible solution with $\mathcal{S}$ and $\mathcal{D}$ as its partite sets.

If $P_1$ and $P_2$ denote paths with vertex sets $\mathcal{S}$ and $\mathcal{D}$ respectively then $T \cup P_1 \cup P_2$ is a tree with attached graphs. Let $Q$ be the incidence matrix of this tree with attached graphs, as defined in Section 2. We may write formulas for the Moore-Penrose inverse of the incidence matrix $Q$ and the inverse of $K = Q^T Q$ using Theorem 2 and Theorem 3 respectively.

We conclude with an example. Consider a transportation problem with 3 sources and 4 destinations. A tableau corresponding to a basic feasible solution and the associated tree with attached graphs (which are paths) are shown in Table 1 and Figure 1 respectively.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
1 & 2 \\
\hline
3 & 4 \\
\hline
5 & 6 \\
\hline
\end{tabular}
\caption{A transportation tableau}
\end{table}
The matrices \( A, B, Q, K \) for \( T \cup P_1 \cup P_2 \), as introduced in Sections 2 and 4, are given by

\[
A = \begin{bmatrix}
1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 \\
-1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 \\
0 & -1 & -1 & 0 & 0 & -1 \\
0 & 0 & 0 & -1 & 0 & 0
\end{bmatrix}, \quad
B = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 \\
-1 & 1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & -1 & 1 & 0 \\
0 & 0 & 0 & -1 & 1 \\
0 & 0 & 0 & 0 & -1
\end{bmatrix}
\]

\[
Q = \begin{bmatrix}
0 & 0 & -1 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 \\
-1 & 1 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 1 & -1 & 0 \\
0 & -1 & -1 & 1 & 0
\end{bmatrix}, \quad
K = Q'Q = \begin{bmatrix}
2 & -1 & 1 & 0 & 1 \\
-1 & 2 & 1 & -1 & -1 \\
1 & 1 & 4 & -2 & 0 \\
0 & -1 & -2 & 2 & 0 \\
1 & -1 & 0 & 0 & 2
\end{bmatrix}
\]

The Moore-Penrose inverse of \( Q \) and the inverse of \( K \) are given by
Note that the number of edges incident to the head-tree and the tail-tree, appearing in Theorems 2 and 3, are very easily seen from the transportation tableau. We leave it to the reader to verify that the expressions for $Q^+$ and $K^{-1}$ given above confirm those given by Theorems 2 and 3.
REFERENCES


