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ON GAUSSIAN ELIMINATION AND DETERMINANT FORMULAS FOR MATRICES WITH CHORDAL INVERSES

MIHÁLY BAKONYI

In this paper a formula is obtained for the entries of the diagonal factor in the UDL factorisation of an invertible operator matrix in the case when its inverse has a chordal graph. As a consequence, in the finite dimensional case a determinant formula is obtained in terms of some key principal minors. After a cancellation process this formula leads to a determinant formula from an earlier paper by W.W. Barrett and C.R. Johnson, deriving in this way a different and shorter proof of their result. Finally, an algorithmic method of constructing minimal vertex separators of chordal graphs is presented.

1. INTRODUCTION AND PRELIMINARIES

Let us introduce first some notations and recall some results. For terminology and results concerning graph theory we follow the book [4]. Let $G = (V, E)$ be an *undirected graph*, where the *vertex set* V is $\{1, \dots, n\}$ and the *edge set* E is a symmetric irreflexive binary relation on V. The *adjacency set* of a vertex v is denoted by $Adj(v)$, that is, $w \in Adj(v)$ if $(v, w) \in E$. Given a subset $A \subseteq V$, define the *subgraph induced* by A by $G_A = (A, E_A)$, where $E_A = \{(x, y) \in E | x \in A \text{ and } y \in A\}$. The *complete graph* is the graph with the property that every pair of distinct vertices is adjacent. A subset $A \subseteq V$ is a *clique* if the induced graph on A is complete. A *path* $[v_1, \dots, v_k]$ is a sequence of vertices such that $(v_j, v_{j+1}) \in E$ for $j = 1, \dots, k-1$. A cycle of length $k > 2$ is a path $[v_1, \dots, v_k, v_1]$ where $v_1, \dots, v_k$ are distinct. A graph G is called *chordal* if every cycle of length stictly greater than 3 possesses a chord, that is, an edge joining two nonconsecutive vertices of the cycle.

An ordering $\sigma = [v_1, \dots, v_n]$ of the vertices of a graph is called *perfect vertex elimination scheme (or perfect scheme)* if each set:

$$X_i = \{v_j \in Adj(v_i) : j > i\} \tag{1.1}$$

is a clique. If a vertex v of G is said to be *simplicial* when $Adj(v)$ is a clique, then σ is a perfect scheme if each v_i is simplicial in the induced graph $G_{\{v_i, \dots, v_n\}}$.

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A subset $S \subseteq V$ is called a *$u-v$ vertex separator* for the nonadjacent vertices u and v if the removal of S from the graph separates u and v into distinct connected components. If no proper subset of S contains a $u-v$ separator, then S is a *minimal $u-v$ separator*. A characterisation given by Fulkerson and Gross [4, Theorem 4.1] asserts: "*A graph G is chordal if and only if G has a perfect scheme, if and only if every minimal vertex separator of G is a clique*".

The *intersection graph* of a family F of nonempty sets is obtained by representing each set in F by a vertex and connecting two vertices by an edge if their corresponding sets intersect. A connected graph with no cycles is called *tree*. The following represents a second characterisation of chordality in [4, Theorem 4.8]: "*A graph $G = (V, E)$ is chordal if and only if there exists a tree $T = (K, E)$ whose vertex set is the set of the maximal cliques of G such that each of the induced subgraphs $T_{K_v} (v \in V)$ is connected (and hence a subtree), where K_v consists of those maximal cliques that contain v*". A tree with this latter property is called *a tree for the graph G*. In general the tree is not uniquely determined by G.

If $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ is a 2×2 operator matrix with A invertible, the operator $D - CA^{-1}B$ is called the *Schur complement* of A in M. Let Ω denote the algebra of matrices $R = (R_{ij})_{i,j=1}^{n}$ where R_{ij} is a (bounded) linear operator acting between the Hilbert spaces H_j and H_i. When $G = (V, E)$ is an undirected graph, denote $\Omega_G = \{R \in \Omega, R_{ij} = 0 \text{ for } (i,j) \notin E\}$.

For an index set $\alpha \subseteq \{1, \ldots, n\}$ and $R \in \Omega$ denote by $R(\alpha)$ the principal submatrix of R corresponding to the index set α.

2. The Results

The next lemma is a simple generalisation of its scalar matrix version in [7]. Since the proof in that paper involves determinants, we present here a modified operator version of it.

Lemma 2.1. *Let G be a chordal graph and $\sigma = [v_1, \ldots, v_n]$ a perfect scheme for G. If $R \in \Omega$ is invertible with $R^{-1} \in \Omega_G$ and the matrices $R(X_k)$ and $R(\{v_k\} \cup X_k)$ are invertible for $k = 1, \ldots, n$, where X_k are given by (1.1), then the matrices $R(\{v_k, \ldots, v_n\})$ are also invertible and $R(\{v_k, \ldots, v_n\})^{-1} \in \Omega_{G_{\{v_k, \ldots, v_n\}}}$ for $k = 2, \ldots, n$.*

Proof: It is sufficient to prove the result for $k = 2$ since after this a simple induction argument proves the result for general k. Let $R = (A_{ij})_{i,j=1}^{3}$ be the block decomposition of R corresponding to the partition $\{v_1\} \cup X_1 \cup \{\{v_2, \ldots, v_n\} - X_1\}$ of the index set V. Let further $R^{-1} = (\alpha_{ij})_{i,j=1}^{3}$ be the correspondently decomposed inverse of R. Since $\alpha_{31} = 0$, the relation:

$$R\begin{pmatrix}\alpha_{11}\\ \alpha_{21}\\ 0\end{pmatrix} = \begin{pmatrix} I\\ 0\\ 0\end{pmatrix}$$

implies that α_{11} is the $(1,1)$ entry of the inverse of $\begin{pmatrix} A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix} = R(\{v_1\}\cup X_1)$. Since $A_{22} = R(X_1)$ is also invertible, it follows that α_{11} is invertible and consequently $\begin{pmatrix} A_{22} & A_{23}\\ A_{23} & A_{33}\end{pmatrix} = R(V - \{v_1\})$ is invertible.

Denote now $R^{-1} = \begin{pmatrix} A & B\\ C & D\end{pmatrix}$ with respect to the partion $\{v_1\}\cup\{v_2,\dots,v_n\}$ of the index set. Then, by the well known Schur complement argument, $R(V - \{v_1\})^{-1} = D - CA^{-1}B$. Let $i,j \neq v_1$ be such that $(i,j) \notin E$. Since $R^{-1} \in \Omega_G$, we have $\left(R(V - \{v_1\})^{-1}\right)_{ij} = -C_{iv_1}A^{-1}_{v_1v_1}B_{v_1j}$. Then v_1 simplicial together with $(i,j) \notin E$ implies that $(i,v_1) \notin E$ or $(j,v_1) \notin E$ and so $C_{iv_1} = 0$ or $B_{v_1j} = 0$. This finishes the proof. ∎

Proposition 2.2. *Let G be chordal and $\sigma = [v_1,\dots,v_n]$ a perfect scheme for G. Assume that $R \in \Omega$ is invertible, $R^{-1} \in \Omega_G$ and $R(X_k)$ and $R(\{v_k\}\cup X_k)$ are invertible for $k = 1,\dots,n$, where X_k are given by (1.1). Denote by $D = (diag(D_k))_{k=1}^{n}$ the diagonal matrix obtained by reducing R by Gaussian elimination with choosing succesively the $(v_1,v_1),\dots,(v_n,v_n)$ diagonal entries to act as pivots. Then D_{v_k} equals the Schur complement of $R(X_k)$ in $R(\{v_k\}\cup X_k)$ for $k = 1,\dots,n$. If the spaces $H_1,\dots,H_n$ are finite dimensional and R satisfies the above conditions then (by the convention $\det R(\emptyset) = 1$)*

$$\prod_{k=1}^{n}\frac{\det M(\{v_k\}\cup X_k)}{\det M(X_k)} \tag{2.1}$$

Proof: Let $M = (A_{ij})_{i,j=1}^{3}$ be an invertible operator matrix with the submatrices $\begin{pmatrix} A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix}$, $\begin{pmatrix} A_{22} & A_{23}\\ A_{32} & A_{33}\end{pmatrix}$, A_{22} invertible. Then a straightforward computation shows that the Schur complement of $\begin{pmatrix} A_{22} & A_{23}\\ A_{32} & A_{33}\end{pmatrix}$ in M equals

$$A_{11} - A_{12}A_{22}^{-1}A_{21} - \left(A_{13} - A_{12}A_{22}^{-1}A_{23}\right)\left(A_{33} - A_{32}A_{22}^{-1}A_{23}\right)^{-1}\left(A_{31} - A_{32}A_{22}^{-1}A_{21}\right) \tag{2.2}$$

In the case when $\left(M^{-1}\right)_{13} = 0$ then $A_{13} = A_{12}A_{22}^{-1}A_{23}$ and when $\left(M^{-1}\right)_{31} = 0$ then $A_{31} = A_{32}A_{22}^{-1}A_{21}$. Each of this equalities imply that (2.2) reduces to $A_{11} - A_{12}A_{22}^{-1}A_{21}$, namely the Schur complement of A_{22} in $\begin{pmatrix} A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix}$.

Apply the above observation to the operator matrix $R(\{v_k,\dots,v_n\})$ written as $(A_{ij})_{i,j=1}^{3}$ with respect to the partition $\{v_k\}\cup X_k\cup\{\{v_{k+1},\dots,v_n\}-X_k\}$ of the index set $\{v_k,\dots,v_n\}$. Since, by Lemma 2.1, the submatrix $R(\{v_{k+1},\dots,v_n\})$ is invertible and the $(1,3)$ and $(3,1)$ entries in the inverse of $M=(A_{ij})_{i,j=1}^{3}$ are 0, then by the previous remark the Schur complement of $R(\{v_{k+1},\dots,v_n\})$ in $R(\{v_k,\dots,v_n\})$ equals the Schur complement of $R(X_k)$ in $R(\{v_k\}\cup X_k)$ for $k=1,\dots,n-1$. By the classical Jacobi result, since $R(\{v_k,\dots,v_n\})$ are invertible, it is possible to reduce the matrix R by Gaussian elimination to the diagonal matrix $D=(diag D_k)_{k=1}^{n}$, by choosing succesively the $(v_1,v_1),\dots,(v_n,v_n)$ diagonal entries of R to act as pivots. Also, D_{v_k} equals the Schur complement of $R(\{v_{k+1},\dots,v_n\})$ in $R(\{v_k,\dots,v_n\})$ and so the first part of the proposition follows. Since in the finite dimensional case the Schur complement of $R(X_k)$ in $R(\{v_k\}\cup X_k)$ equals $(\det R(\{v_k\}\cup X_k)/(\det R(X_k)))$, formula (2.1) is a consequence of $\det R=\det D$. ∎

We remark that without loss of generality in the previous proposition it can be assumed that $\sigma=[1,\dots,n]$ since otherwise we reorder the rows and columns of R by the ordering of σ, and under this assumption D is the diagonal factor in the UDL factorisation of R.

The rest of the paper deals with determinant formulas and thus all the spaces are assumed to be finite dimensional. In the paper [2], it is proved that if G is chordal, $T=(V(G),E(G))$ is a tree for G, $R\in\Omega$ is invertible with $R^{-1}\in\Omega_G$, then

$$\det R=\frac{\prod_{V\in V(G)}\det R(V)}{\prod_{\{V_1,V_2\}\in E(G)}\det R(V_1\cap V_2)} \tag{2.3}$$

provided that the terms of the denominator are nonzero.

Next we present how the formula (2.3) can be obtained from (2.1).

Proposition 2.3. *For any perfect scheme $\sigma=[v_1,\dots,v_n]$ and tree $T=(V(T),E(T))$ for G the formula (2.3) can be obtained from (2.1) by cancellation.*

Proof: The proposition is proven by induction on n, the number of vertices of G. For $n=1$ it is obvious. Suppose now that $T'=(V(T'),\,E(T'))$ is a tree for the graph $G_{\{v_2,\dots,v_n\}}$. Assume that

$$\prod_{k=2}^{n}\frac{\det M(\{v_k\}\cup X_k)}{\det M(X_k)}=\frac{\prod_{W\in V(T')}\det M(W)}{\prod_{(W,W')\in E(T)}\det M(W\cap W')}. \tag{2.4}$$

There are two possibilities:

A. The clique X_1 is not maximal in $G_{\{v_2,\dots,v_n\}}$. Then a tree $T=(V(T),\,E(T))$ can be obtained by adding to $V(T')$ a new vertex corresponding to $\{v_1\}\cup X_1$ and a new edge joining this vertex with the vertex of $V(T')$ corresponding to the maximal clique of $G_{\{v_2,\dots,v_n\}}$ containing X_1.

Thus

$$\frac{\prod_{W\in V(T)} \det M(W)}{\prod_{(W,W')\in E(T)} \det M(W\cap W')} = \frac{\det M(\{v_1\}\cup X_1)}{\det M(X_1)} \frac{\prod_{W\in V(T')} \det M(W)}{\prod_{(W,W')\in E(T')} \det M(W\cap W')}$$

and the equality is proved for G without any new cancellation.

B. The clique X_1 is maximal in $G_{\{v_2,\dots,v_n\}}$. A tree $T = (V(T),\, E(T))$ for G can be obtained from T' by renaming the vertex corresponding to X_1 by $\{v_1\}\cup X_1$.

Thus, in the product

$$\frac{\det M(\{v_1\}\cup X_1)}{\det M(X_1)} \prod_{k=2}^{n} \frac{\det M(\{v_k\}\cup X_k)}{\det M(X_k)}$$

the term $\det M(X_1)$ will be cancelled.The right member of (2.4) after multiplication with $(\det M(\{v_1\}\cup X_1))/(\det M(X_1))$ and cancellation of $\det M(X_1)$ becomes $\left(\prod_{W\in V(T)} \det M(W)\right)/\left(\prod_{(W,W')\in E(T)} \det M(W\cap W')\right)$. The denominator of this latter expression coincides with the denominator of (2.3) since v_1 is contained in a unique maximal clique of V. This finishes the proof. $\square$

In [**3**, Theorem 3.5] it is proved that for any tree T for G, the set of cliques appearing in the denominator of (2.3) is the set of minimal vertex separators of the graph G. From Proposition 2.3, it follows that for any perfect scheme $\sigma = [v_1,\dots,v_n]$ of G, in the denominator of (2.3) appear the cliques of the form X_i which are not maximal in $G_{\{v_{i+1},\dots,v_n\}}$. The following result can be obtained as a consequence of [**3**, Proposition 2.3 and Theorem 3.5] but it can be proved also directly. It represents an algorithmic method of constructing the minimal vertex separators of a chordal graph.

Proposition 2.4. *Let $G = (V,E)$ be a chordal graph and $\sigma = [v_1,\dots,v_n]$ a perfect scheme for G. A subset $S \subseteq V$ is a minimal vertex separator of G if and only if S equals some X_i $(i < n)$ that is not a maximal clique in $G_{\{v_{i+1},\dots,v_n\}}$.*

Proof: The proposition is proven by induction on the cardinality of V. For $n \leqslant 3$ it is immediate. Assume that it holds for $G' = G_{\{v_2,\dots,v_n\}}$.

Since v_1 is simplicial any minimal $v_k - v_m$ separator is the same in G' and G for any $k, m \geqslant 2$. If X_1 is not maximal in G' then there exists a vertex $v_m, m \geqslant 2$, with $X_1 \subseteq Adj(v_m)$, so X_1 is a minimal $v_1 - v_m$ separator. Conversely, if X_1 is a minimal vertex separator in G, by [4, Exercise 12, p.102] X_1 is not maximal in G'. After removing any $v_1 - v_k$ separator from G, different from X_1, the connected component of v_1 must contain a vertex v_r, $r \geqslant 2$. Since v_1 is simplicial, our minimal $v_1 - v_k$

separator must coincide with a minimal $v_r - v_k$ separator and by the assumption made for G' it is of the desired form. So the statement is completely proved. $\square$

If R is a partial positive definite matrix (see [5] for definitions) then in [5] it was proved that there is a unique positive definite completion Q of R with the property that $\left(Q^{-1}\right)_{ij} = 0$ for the entries (i,j) for which R_{ij} is unknown. Also Q represents the unique maximum determinant positive definite completion of R. Then, if in addition the graph G of R is chordal, $\det Q$ can be obtained by the formula (2.3). This was proved in [6]. In [3], another formula for $\det Q$ was given. In [1] a formula for the determinant of an arbitrary positive definite completion of R was given.

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Department of Mathematics
The College of William and Mary
Williamsburg VA 23187-8795
United States of America

Present address:
Department of Mathematics
Georgia State University
Atlanta, GA 30303
United States of America