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SELECTED TOPICS IN MATRIX ANALYSIS

A Thesis

Presented to

The Faculty of the Department of Mathematics

San Jose State University

In Partial Fulfillment
of the Requirements for the Degree
Master of Science

by Winston W. Wheeler May 1996 UMI Number: 1379388

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ABSTRACT

SELECTED TOPICS IN MATRIX ANALYSIS

by Winston W. Wheeler

In the first part of this thesis, properties of Hadamard matrices and symmetric block designs are proved and applied to establish the growth factor for Hadamard matrices through size 12×12 . Growth is proportional to the maximum pivot size when a matrix is reduced by Gaussian elimination with complete pivoting, and is of interest because it is one of the factors in error bounds for calculated solutions of linear systems.

The second part of this thesis studies the problem of which partial Hermitian matrices (some entries specified, some free) can be completed to positive definite matrices. The undirected graph of the specified entries is chordal if and only if every partial positive definite matrix with that graph can be completed. When a positive definite completion exists, the inverse of the completion with maximum determinant has zeros in those positions corresponding to unspecified entries in the original partial Hermitian matrix.

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PART ONE

GROWTH IN GAUSSIAN ELIMINATION IN HADAMARD MATRICES

CHAPTER 1

BACKGROUND

In the following work, we will give explicit citations for theorems when possible. However, for convenience here, some of our theorems amalgamate well-known results from basic matrix theory. This material can be found in books such as [HJ].

1.1 Hadamard Matrices

1.1.1 <u>Definition</u>. An $n \times n$ Hadamard matrix H is a matrix whose entries are ± 1 and $HH^t = nI$.

Notice this implies that the rows are pairwise orthogonal.

- 1.1.2 By the following theorem, the columns of a Hadamard matrix are also pairwise orthogonal. Thus the transpose of a Hadamard matrix is also Hadamard.
- **1.1.3** Theorem. If H is an $n \times n$ Hadamard matrix, then $|\det(H)| = n^{n/2}$ and $H^{-1} = (1/n)H^{t}$. Thus H is normal.

Proof. Since $[\det(H)]^2 = \det(H)\det(H^t) = \det(HH^t) = \det(nI) = n^n$, $|\det(H)| = n^{n/2}$. Hence H is invertible. In addition, since $HH^t = nI$, we also have $H^{-1} = (1/n)H^t$.

So $H^{t}H = nH^{-1}H = nI = HH^{t}$, i.e., H is (real) normal.

1.1.4 <u>Proposition</u>. Suppose H is Hadamard. If any one or more of the following operations is done to H, the resulting matrix is again Hadamard:

- 1) Rearrange rows
- 2) Rearrange columns
- 3) Scale any row by -1
- 4) Scale any column by -1.

Proof. One row (or column) exchange still results in a matrix with pairwise orthogonal rows (or columns). Any row (column) scaled by -1 is still orthogonal to every other row (column).

1.1.5 <u>Definition</u>. If H is Hadamard and H_1 is obtained from H as described in the proposition above, then H and H_1 are called *Hadamard equivalent*.

We have come across three different proofs of the well-known fact that the size p of a Hadamard matrix must be a multiple of four if p > 2: Hadamard's original proof, one by Paley, and one found in [DP]. It is interesting how different the proofs are. They illustrate the remarkable variety of ideas people have employed in the study of Hadamard matrices, so we present each one.

1.1.6 Theorem. The matrices [1] and $\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$ are Hadamard. If H is a $p \times p$

Hadamard matrix and p > 2, then p is a multiple of four.

First proof [Had]. By Proposition 1.1.4, we can scale columns of H to create a Hadamard equivalent matrix H_1 whose first row entries are all +1. Next, we can rearrange columns of H_1 to obtain a Hadamard equivalent matrix H_2 whose second row looks like [1...1 -1...-1]. Finally, rearrange columns of H_2 to obtain a Hadamard equivalent matrix H_3 whose third row looks like [1...1 -1...-1 1...-1]. In row three of H_3 , let a = the number of +1 entries that occur below +1 entries in row two. Let b = the number of -1 entries that occur below -1 entries in row two. And let d = the number of -1 entries that occur below -1 entries in row two.

Because row two is orthogonal to row one, there must be an even number of columns, i.e., p is even. Since p > 2, let p = 2k for some integer k > 1. Then there are k positive entries in row two and k negative entries in row two. Thus a + b = c + d = k. Because rows two and three are orthogonal, we must have b + c = a + d = k. In addition, because rows one and three are orthogonal, we must have a + c = b + d = k. Hence a + b = a + c = b + c = b + d so that a = b = c = d. Thus b + c = k implies 2b = k. Therefore, p = 2(2b), i.e., p is a multiple of four.

Second proof [DP]. Because the rows are pairwise orthogonal, there must be an even number of columns. Hence p = 2k for some integer k > 1 since p > 2. By Theorem 1.1.3, $|det(H)| = (2k)^k$.

By Proposition 1.1.4, we can scale rows and columns of H by ± 1 to create a Hadamard equivalent matrix H_1 whose first row and column are all ± 1 . Subtract row 1 of H_1 from each of rows 2 through p, obtaining $\begin{bmatrix} 1 & z \\ 0 & A \end{bmatrix}$, where $z = \begin{bmatrix} 1 & ... 1 \end{bmatrix}$ and A is a $(p-1) \times (p-1)$ matrix whose entries are 0 and -2. Since neither scaling rows and columns by ± 1 nor adding multiples of one row to other rows affects the magnitude of the determinant, we have $|\det(H_1)| = |\det(H_1)| = |\det(A)| = 2^{p-1} |\det(B_1)|$, where B is a 0, -1

matrix. Since det(B) must be an integer, we have $(2k)^k = |det(H)| = 2^{2k-1}n$, where n is an integer; therefore $k^k/2^{(k-1)}$ is an integer, which can happen only if k is even. Since we already have p = 2k, we conclude that p is a multiple of four.

Third proof [Pal]. Let $H = [h_{ij}]$. For $k \in \{1, 2, ..., p\}$, let h_k denote the kth row of H. Since the rows of H are pairwise orthogonal, $(h_1 + h_2) \cdot (h_1 + h_3) = h_1 \cdot h_1 + h_1 \cdot h_3 + h_2 \cdot h_1 + h_2 \cdot h_3 = h_1 \cdot h_1 = p$. Since both $h_1 + h_2$ and $h_1 + h_3$ are $0, \pm 2$ vectors, the product of their ith components, $(h_{1i} + h_{2i})(h_{1i} + h_{3i})$, is 0 or 4. Hence $(h_1 + h_2) \cdot (h_1 + h_3)$ is a multiple of four, i.e., p is a multiple of four.

1.1.7 Theorem. [Had] (Hadamard's Inequality) Let $A = [a_{ij}]$ be an $n \times n$ real matrix with $|a_{ij}| \le 1$ for all $i, j \in \{1, ..., n\}$. Then $|det(A)| \le n^{n/2}$, and equality holds if and only if A is Hadamard.

Proof. Let x_i denote column i of A. We first show that $\det(A^tA) \leq \prod_{i=1}^n (x_i^tx_i)$, with equality holding if and only if the columns of A are pairwise orthogonal.

First suppose the columns of A are pairwise orthogonal. Then because

$$A^{t}A = \begin{bmatrix} (x_{1}^{t}x_{1}) & (x_{1}^{t}x_{2}) & \dots & (x_{1}^{t}x_{n}) \\ (x_{2}^{t}x_{1}) & (x_{2}^{t}x_{2}) & \dots & (x_{2}^{t}x_{n}) \\ \vdots & \vdots & \ddots & \vdots \\ (x_{n}^{t}x_{1}) & (x_{n}^{t}x_{2}) & \dots & (x_{n}^{t}x_{n}) \end{bmatrix}$$
which is diagonal when the columns of A

are pairwise orthogonal, $det(A^tA) = \prod_{i=1}^{n} (x_i^t x_i)$.

Now suppose the columns of A are not pairwise orthogonal. We will show that $\det(A^tA) < \prod_{i=1}^n (x_i^t x_i^t). \tag{1}$

We proceed by induction on n, the size of A. Suppose n = 2 and x_1 and x_2 are not orthogonal. Then $(x_1^t x_2) = (x_2^t x_1) \neq 0$. Hence

$$\det(\mathbf{A}^{t}\mathbf{A}) = \det\begin{bmatrix} \mathbf{x}_{1}^{t}\mathbf{x}_{1} & \mathbf{x}_{1}^{t}\mathbf{x}_{2} \\ \mathbf{x}_{2}^{t}\mathbf{x}_{1} & \mathbf{x}_{2}^{t}\mathbf{x}_{2} \end{bmatrix} < (\mathbf{x}_{1}^{t}\mathbf{x}_{1})(\mathbf{x}_{2}^{t}\mathbf{x}_{2}).$$

Now let $n \ge 3$ and suppose (1) is true through size n-1. Let A be $n \times n$ with columns x_1, \ldots, x_n such that at least two of them are not orthogonal to each other. Since $n \ge 3$, we may rearrange the columns so that two of the first n-1 columns are not orthogonal. At most this changes the sign of the determinant of A, hence does not affect $\det(A^tA)$. So let $A = [x_1 \dots x_n]$ represent this possibly new matrix. Let U be a real orthogonal matrix such that $UA = \begin{bmatrix} A_1 & y \\ 0 & c \end{bmatrix}$, where A_1 is $(n-1) \times (n-1)$.

(The idea is to rotate \mathbb{R}^n so that the span of the first n-1 columns of A goes into $\mathbb{R}^{n-1} \times \{0\}$. For example, the QR factorization of A would supply an orthogonal matrix which yields such a mapping: $A = \mathbb{Q}\mathbb{R}$, Q orthogonal and R upper triangular implies $\mathbb{Q}^t A = \mathbb{R}$ [HJ, 2.6.1].)

Let
$$y_i$$
 denote column i of A_1 . Then $UA = [Ux_1...Ux_{n-1} \ Ux_n] = \begin{bmatrix} y_1 & ... & y_{n-1} & y \\ 0 & ... & 0 & c \end{bmatrix}$.
So if $i, j \in \{1,..., n-1\}$, we have $x_i^t x_j = x_i^t U^t Ux_j = (Ux_i)^t (Ux_j) = y_i^t y_j$. Thus since

 $x_1,..., x_{n-1}$ are not pairwise orthogonal, the columns of A_1 are not pairwise orthogonal. By the inductive hypothesis, $\det(A_1^tA_1) < \prod_{i=1}^{n-1} (y_i^ty_i)$. Now we have

$$\begin{split} \det(A^t A) &= \det[(UA)^t (UA)] = \det \begin{bmatrix} A_1^t & 0 \\ y^t & c \end{bmatrix} \det \begin{bmatrix} A_1 & y \\ 0 & c \end{bmatrix} = c \cdot \det(A_1^t) \cdot c \cdot \det(A_1) = \\ c^2 \det(A_1^t A_1) &< c^2 \prod_{i=1}^{n-1} (y_i^t y_i) = c^2 \prod_{i=1}^{n-1} (x_i^t x_i) \leq \prod_{i=1}^{n} (x_i^t x_i) \text{ since } x_n^t x_n = y^t y + c^2. \end{split}$$

This completes the proof of (1). Thus we have shown that $\det(A^tA) \leq \prod_{i=1}^n (x_i^t x_i)$, and equality holds if and only if the columns of A are pairwise orthogonal.

We now notice that $\prod_{i=1}^n (x_i^t x_i) = n^n$ if $|a_{ij}| = 1$ for all i and j, and is strictly less otherwise. (Recall that $|a_{ij}| \le 1$ for all i and j.) In other words, $\prod_{i=1}^n (x_i^t x_i) \le n^n$, with equality holding if and only if $|a_{ij}| = 1$ for all i and j. Thus we have shown that $\det(A^t A) \le n^n$, and equality holds if and only if A is Hadamard. Hadamard's Inequality then follows immediately.

1.2 Symmetric Block Designs and Hadamard Matrices

1.2.1 <u>Definition</u>. A symmetric block design with parameters v, k and λ , or (v, k, λ) -symmetric block design, is a collection of v objects and v sets (called blocks) such that

•every block contains k objects,

•every object is found in k blocks,

•every pair of blocks has λ objects in common, and

•every pair of objects occurs together in exactly λ blocks.

1.2.2 <u>Definition</u>. An *incidence matrix* of a (v, k, λ) -symmetric block design is a $v \times v$ matrix defined as follows: Number the objects 1 through v and number the blocks 1 through v. Define $A = [a_{ij}]$ by

 $a_{ij} = 1$ if object i belongs to block j, and

 $a_{ij} = 0$ otherwise.

1.2.3 Remark. A different numbering of objects and/or blocks would yield an incidence matrix which could be obtained from A by permuting rows and/or columns. It is often useful to associate each row of A with an object and each column with a block.

The following theorem is essentially due to Todd [Tod]. He stated it somewhat differently as symmetric block designs had not yet been defined.

1.2.4 Theorem. There exists a (4n-1, 2n-1, n-1)-symmetric block design if and only if there exists a $4n \times 4n$ Hadamard matrix.

Proof. (\Leftarrow) Let H be a Hadamard matrix of order 4n. Negate rows and columns as necessary so that the first row and column of the resulting matrix H_1 are positive. By Proposition 1.1.4, H_1 is Hadamard. Define a $(4n-1) \times (4n-1)$ matrix B by deleting the first row and column of H_1 and changing every -1 in the remaining submatrix to 0. Then B can be thought of as an incidence matrix if we identify each row with one object and each column with one block. We will show that B is an incidence matrix of a (4n-1, 2n-1, n-1)-symmetric block design.

Since H₁ is Hadamard and each entry of column 1 and row 1 is +1, each of columns 2 through 4n and each of rows 2 through 4n of H₁ contains +1 in exactly 2n positions. Hence there are 2n-1 positive entries in each column and in each row of B. So it follows that each block contains 2n-1 objects and each object is found in 2n-1 blocks. Now we need only show that any 2 objects occur together in exactly n-1 blocks and any 2 blocks have n-1 objects in common. That is, if we choose any two rows (columns) of B, there will be exactly n-1 positions where +1 appears in both rows (columns), i.e., their dot product will be n-1. We include the proof for rows of B; the proof for columns is similar.

Let i, $j \in \{2,...,4n\}$ with $i \neq j$. We will show that there are n positions where +1 occurs in both row i and row j of H_1 . Suppose there are k positions where +1 occurs in both rows. Then there are 2n-k other +1's in row i matched with -1 in row j, and 2n-k other +1's in row j matched with -1 in row i. Hence the dot product of row i with row j will include 4n-2k occurrences of -1 which implies that k = n since row i and row j are orthogonal. Since B is obtained by deleting the first row and column of H_1 and changing every -1 in the remaining submatrix to 0, for any two rows of B, there are n-1 positions where +1 appears in both rows, i.e., their dot product is n-1.

By a similar argument for columns, we conclude that for any two columns of B, there are n-1 positions where +1 occurs in both columns. Therefore we have shown that B is an incidence matrix of a (4n-1, 2n-1, n-1)-symmetric block design.

We remark that the definition of B given above may seem arbitrary, but it actually arises rather naturally. The matrix B in this theorem is essentially the "reverse" of the matrix we called B in the second proof of Theorem 1.1.6, where by "reverse" we mean change each 0 to 1 and each -1 to 0.

(⇒) Let B be an incidence matrix of a (4n-1, 2n-1, n-1)-symmetric block design. Then B has order 4n-1, each row of B has (2n-1) +1's and 2n 0's, and the dot product of any two rows is n-1. Let i, j ∈ {1,..., 4n-1} with i ≠ j. Then in row i of B, there are n-1 positions where +1 occurs matched with +1 in row j of B. Also in row i of B, there are (2n-1)-(n-1) = n positions where +1 occurs matched with 0 in row j of B. Thus in row i of B, there are 2n-n = n positions where 0 occurs matched with 0 in row j, and hence n positions where 0 occurs matched with +1 in row j. Adjoin to B a first column and first row of all +1's, obtaining the $4n \times 4n$ matrix $\begin{bmatrix} 1 & z \\ z^t & B \end{bmatrix}$, where z = [1...1]. Change the 0's in B to -1's. We will show that the resulting matrix H is Hadamard.

Since H is a ± 1 matrix, we need only show that any two rows of H are orthogonal. In each of rows 2 through 4n of H, there are 2n occurrences of +1 and 2n occurrences of -1. Hence row 1 of H is orthogonal to every other row. Let i, $j \in \{2,...,4n\}$ with $i \neq j$. Then from what we know about B above, there are n positions in row i of H where +1 appears matched with +1 in row j, n positions where +1 appears matched with -1 in row j, n positions where -1 appears matched with -1 in row j. Hence the dot product of row i with row j is zero, i.e., row i and row j are orthogonal. Since the choice of i and j was arbitrary, we conclude that any two

rows of H selected from rows 2 through 4n are orthogonal. Thus we have shown that the rows of H are pairwise orthogonal, and H is Hadamard.

1.2.5 Example. The existence of a 12×12 Hadamard matrix is equivalent to the existence of an (11, 5, 2)-symmetric block design.

where + denotes a + 1 entry and - denotes a - 1 entry.

Therefore

where + denotes a + 1 entry.

Let row i of B correspond to object i; let column i of B correspond to block i, and let B_i denote block i. Then

$$B_1 = \{1, 4, 8, 9, 10\}; \qquad B_2 = \{2, 5, 9, 10, 11\}; \qquad B_3 = \{1, 3, 6, 10, 11\}; \\ B_4 = \{1, 2, 4, 7, 11\}; \qquad B_5 = \{1, 2, 3, 5, 8\}; \qquad B_6 = \{2, 3, 4, 6, 9\}; \\ B_7 = \{3, 4, 5, 7, 10\}; \qquad B_8 = \{4, 5, 6, 8, 11\}; \qquad B_9 = \{1, 5, 6, 7, 9\}; \\ B_{10} = \{2, 6, 7, 8, 10\}; \qquad B_{11} = \{3, 7, 8, 9, 11\}.$$

There are 11 objects. Each block has 5 objects, and it is easy to check that each object is found in 5 blocks. Furthermore, a straightforward check shows that each pair of objects occurs together in exactly 2 blocks, and that each pair of blocks has two objects in common. The construction is reversible, and so the equivalence follows.

1.3 Gaussian Elimination

"Gaussian elimination" is defined somewhat differently by different authors. We need to have a very explicit meaning for the term. Informally, our definition of usual Gaussian elimination is: Use replace-type row operations to reduce the matrix, with no row or column exchanges unless necessary to obtain a nonzero value in the next diagonal position. The formal definition follows.

- **1.3.1** <u>Definitions.</u> Let $A = [a_{ij}]$ be a nonzero $n \times n$ real matrix. In this paper, to reduce A by usual Gaussian elimination means perform the following steps:
- (1) If $a_{11} = 0$, choose some $a_{kp} \neq 0$ and exchange rows 1 and k and columns 1 and p to get the nonzero entry in the (1, 1) position. Let $A^{(0)} = \left[a_{ij}^{(0)}\right]$ denote the new matrix.
- (2) Pivot on $a_{11}^{(0)}$ --that is, add multiples of row 1 to the rows below it to create zeros in their column 1 positions. Let

$$A^{(1)} = \begin{bmatrix} a_{11}^{(0)} & a_{12}^{(0)} & a_{13}^{(0)} & \dots & a_{1n}^{(0)} \\ 0 & a_{22}^{(1)} & a_{23}^{(1)} & \dots & a_{2n}^{(1)} \\ 0 & a_{32}^{(1)} & a_{33}^{(1)} & \dots & a_{3n}^{(1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & a_{n3}^{(1)} & \dots & a_{nn}^{(1)} \end{bmatrix}$$

be the new matrix obtained.

(3) For each k = 2,..., n-1, repeat steps (1) and (2) on the $(n-k+1) \times (n-k+1)$ lower right principal submatrix of $A^{(k-1)}$, as long as that submatrix is not all zero. The final matrix will be upper triangular and will be denoted as follows:

$$A^{(n-1)} = \begin{bmatrix} a_{11}^{(0)} & a_{12}^{(0)} & a_{13}^{(0)} & \dots & a_{1n}^{(0)} \\ 0 & a_{22}^{(1)} & a_{23}^{(1)} & \dots & a_{2n}^{(1)} \\ 0 & 0 & a_{33}^{(2)} & \dots & a_{3n}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & a_{nn}^{(n-1)} \end{bmatrix}.$$

We will call the diagonal entries *pivots*. We often use p_k to denote $\left|a_{kk}^{(k-1)}\right|$, the magnitude of the kth pivot.

- **1.3.2** If the algorithm can be completed without any row or column exchanges, i.e., if for each $k \in \{1, ..., n-1\}$, $a_{kk}^{(k-1)} \neq 0$ when $A^{(k-1)}$ is created, then we will say that A has Property P.
- 1.3.3 In numerical algorithms, step (1) in 1.3.1 is often modified so that even when $a_{kk}^{(k-1)} \neq 0$ when $A^{(k-1)}$ is created, a row and/or column exchange may be done in the $(n-k+1) \times (n-k+1)$ trailing principal submatrix of $A^{(k-1)}$ so that some other number is used for the kth pivot. The criteria for choosing the next pivot is called a *pivoting strategy*. We are interested here in the pivoting strategy called *Gaussian elimination with complete pivoting (GECP)*. The algorithm is the same as the one for usual Gaussian elimination, except we replace step (1) with the following:
- (1') Search column 1 from row 1 to n, then columns 2,..., n in the same way, for an entry with maximal magnitude. Using the <u>first</u> such a_{kp} found, exchange rows 1 and k and columns 1 and p, if necessary, to put a_{kp} into the (1, 1) position. Let $A^{(0)} = \left[a_{ij}^{(0)}\right]$ denote the new matrix.

1.3.4 Theorem. An $n \times n$ real matrix A is invertible if and only if every pivot is nonzero.

Proof. The only matrix operations involved in usual Gaussian elimination or GECP are adding multiples of a row to other rows, and row and column exchanges, both of which leave the magnitude of the determinant unchanged. Thus $|\det(A)| = |\det(A^{(n-1)})| = |a_{11}^{(0)}a_{22}^{(1)}\cdots a_{nn}^{(n-1)}|$. Hence A is invertible if and only if every pivot is nonzero.

1.3.5 <u>Definition</u>. Matrices which require no row or column exchanges during GECP will be called *completely pivoted (CP)*.

1.3.6 Example.
$$A = \begin{bmatrix} 1 & 1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & 3 \end{bmatrix}$$
 has Property P, but is not CP.

1.3.7 It is observed in [DP] that any $n \times n$ matrix A can easily be altered to obtain a new matrix B which is CP and for which $B^{(n-1)} = A^{(n-1)}$. To get B, imagine that GECP is done to A and one keeps track of the row and column exchanges that occur. Do these exchanges to A first, in the same order, and call the resulting matrix B. Then GECP on B would not require any exchanges, and $A^{(n-1)} = B^{(n-1)}$.

1.3.8 Example. Do GECP on

Observe that we exchanged rows 2 and 3 of $H^{(1)}$, rows 3 and 4 of $H^{(2)}$, and rows 4 and 6 and columns 4 and 5 of $H^{(3)}$. If we perform these exchanges to H first, in the same order they occurred during GECP on H, we obtain

Performing GECP on B results in no row or column exchanges, and at its conclusion we get

$$B^{(7)} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -2 & 0 & -2 & 0 & 0 & -2 & -2 \\ 0 & 0 & -2 & 2 & 0 & -2 & 2 & 0 \\ 0 & 0 & 0 & -4 & -2 & 2 & -2 & -2 \\ 0 & 0 & 0 & 0 & -2 & 2 & -2 & 2 \\ 0 & 0 & 0 & 0 & 0 & -4 & 0 & -4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 \end{bmatrix} = H^{(7)}.$$

CHAPTER 2

MAIN RESULTS

2.1 Properties concerning Determinants

2.1.1 <u>Definition</u>. Let A be an $n \times n$ real matrix. $A(i_1...i_p|j_1...j_p)$ will denote the $p \times p$ submatrix of A obtained from the intersection of rows $i_1,...,i_p$ with columns $j_1,...,j_p$. When the two sets of indices are the same, $A(i_1...i_p)$ will abbreviate except for the following two cases:

A(p) will denote the leading $p \times p$ principal submatrix of A, i.e., A(1...p), and A[p] will denote the trailing $p \times p$ principal submatrix of A, i.e., A(n-p+1...n).

This notation is similar to that in [HJ]. It is different from the notations found in the three main references for this chapter, [DP], [EM], and [Gan]. Each of these uses a different notation: In [DP], $A(i_1...i_p|j_1...j_p)$ denotes a determinant; [Gan] uses a similar notation for determinants; and in [EM], A(p) and A[p] both denote magnitudes of determinants.

2.1.2 Theorem. [Gan, p. 26] Suppose A is $n \times n$, invertible, has Property P, usual Gaussian elimination is done on A, and $1 \le k < n$. Then if k < i, j,

$$a_{ij}^{(k)} = \frac{\det A(1...k il1...k j)}{\det A(k)}.$$

Thus the kth pivot, $a_{kk}^{(k-1)} = \det A(k)/\det A(k-1)$.

Proof. Because A has Property P, both A(k) and A(1...k il1...k j) do also. Since the determinant of a matrix is unchanged by adding multiples of a row to other rows, we have det A(1...k il1...k j) = det A^(k)(1...k il1...k j) = $a_{11}^{(0)}a_{22}^{(1)}\cdots a_{kk}^{(k-1)}a_{ij}^{(k)}$, and det A(k) = $a_{11}^{(0)}a_{22}^{(1)}\cdots a_{kk}^{(k-1)}$. By Theorem 1.3.4, since A is invertible, every pivot is nonzero. Hence det A(k) \neq 0. So we have

$$a_{ij}^{(k)} = \frac{a_{11}^{(0)} a_{22}^{(1)} \cdots a_{kk}^{(k-1)} a_{ij}^{(k)}}{a_{11}^{(0)} a_{22}^{(1)} \cdots a_{kk}^{(k-1)}} = \frac{\det A(1...k \ ii1...k \ j)}{\det A(k)}.$$

Observe that the same result is true if A is invertible, CP, and GECP is done on A.

- **2.1.3** Remark. In the course of proving Theorem 2.1.2, we have also shown that any leading principal submatrix of an invertible matrix with Property P is invertible.
- **2.1.4** <u>Definition</u>. Let $A = [a_{rs}]$ be an $n \times n$ real matrix. The *adjugate of A*, denoted by adj(A), is the transpose of the matrix of cofactors of the elements a_{rs} of A, i.e., if $r, s \in \{1, ..., n\}$, the (s, r)-entry of adj(A) is $(-1)^{r+s} \det A(1...\hat{r}...n|1...\hat{s}...n)$, where \hat{r} means "omit r."
- **2.1.5** Theorem. [Lip, p. 176] Suppose A is an $n \times n$ invertible real matrix. Then

$$A^{-1} = \frac{1}{\det(A)} \cdot \operatorname{adj}(A).$$

- **2.1.6** Theorem. [DP] Suppose A is $n \times n$, invertible, has Property P, usual Gaussian elimination is done on A, and $1 \le k \le n$. Then the kth pivot $a_{kk}^{(k-1)}$ is 1/x where x is the (k, k)-entry of $A(k)^{-1}$. In particular, this theorem is true if A is CP.
- Proof. By 2.1.3, A(k) is invertible. Let B = A(k). Then by Theorem 2.1.5, the (k, k)-entry of B⁻¹ is $\frac{\det B(k-1)}{\det(B)}$, and this equals $\frac{\det A(k-1)}{\det A(k)}$ which equals $1/a_{kk}^{(k-1)}$ by

Theorem 2.1.2.

- **2.1.7** Corollary. [Tor], [Cry] If H is an $n \times n$ Hadamard matrix and H is reduced to upper triangular form with any pivoting strategy, then the final pivot has magnitude n. Proof. Whatever pivoting strategy is used, we may assume the row and column exchanges involved are done to H first. Then the new matrix H_1 has Property P, and is Hadamard by Proposition 1.1.4. By Theorem 2.1.6, the final pivot of H_1 is 1/x where x is the (n, n)-entry of $H_1^{-1} = (1/n)H_1^{-1}$. Hence $x = \pm 1/n$ which implies that the final pivot is $\pm n$.
- **2.1.8** Theorem. [Gan, p. 21] Let M be an $n \times n$ invertible matrix and let $1 \le k < n$. If $\alpha = \{i_1 < i_2 < \cdots < i_k\}$ is an ordered subset of $\{1, 2, \ldots, n\}$, let $\alpha' = \{i_1' < i_2' < \cdots < i_{n-k}'\}$ denote its ordered complement. Then for any ordered subsets $\alpha = \{i_1 < i_2 < \cdots < i_k\}$ and $\beta = \{j_1 < j_2 < \cdots < j_k\} \subset \{1, 2, \ldots, n\}$,

$$\begin{split} \det M^{-1}(i_1...i_k|j_1...j_k) &= \frac{\left(-1\right)^m}{\det(M)} \det \ M(j_1'...j_{n\cdot k}'|i_1'...i_{n\cdot k}') \\ \text{where } m &= \sum_{r=1}^k (i_r + j_r). \end{split}$$

We first prove the following:

2.1.9 Lemma. Let $X = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$, where D is a k×k block and A is (n-k)×(n-k).

Suppose X is invertible and $X^{-1} = \begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix}$, where D_1 is a $k \times k$ block. Then

$$\det(D_1) = \frac{\det(A)}{\det(X)}, \text{ i.e., } \det X^{-1}[k] = \frac{\det X(n-k)}{\det(X)}.$$

Proof. We first show that A is invertible if and only if D_1 is invertible.

Suppose A is invertible. Then
$$\begin{bmatrix} A & B \\ 0 & D - CA^{-1}B \end{bmatrix} = \begin{bmatrix} I & 0 \\ -CA^{-1} & I \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$
 is the product of

invertible matrices, hence is invertible. Thus D-CA-1B is invertible. Now

$$\begin{bmatrix} A^{-1} & 0 \\ 0 & (D-CA^{-1}B)^{-1} \end{bmatrix} \begin{bmatrix} I & -B(D-CA^{-1}B)^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} A & B \\ 0 & D-CA^{-1}B \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \text{ which }$$
 implies that
$$\begin{bmatrix} A^{-1} & 0 \\ 0 & (D-CA^{-1}B)^{-1} \end{bmatrix} \begin{bmatrix} I & -B(D-CA^{-1}B)^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ -CA^{-1} & I \end{bmatrix} = X^{-1} \text{ which is }$$

$$\begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix} \text{ by definition. Thus } D_1 = (D-CA^{-1}B)^{-1}, \text{ i.e., } D_1 \text{ is invertible. (§)}$$

To prove the converse, suppose D_1 is invertible. Then

$$\begin{bmatrix} A_1 - B_1 D_1^{-1} C_1 & 0 \\ D_1^{-1} C_1 & I \end{bmatrix} = \begin{bmatrix} I & -B_1 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & D_1^{-1} \end{bmatrix} \begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix}$$
 is the product of invertible matrices,

hence is invertible. Thus $A_1 - B_1 D_1^{-1} C_1$ is invertible. Now

$$\begin{bmatrix} I & 0 \\ -D_1^{-1}C_1 & I \end{bmatrix} \begin{bmatrix} (A_1 - B_1D_1^{-1}C_1)^{-1} & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} A_1 - B_1D_1^{-1}C_1 & 0 \\ D_1^{-1}C_1 & I \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \text{ which implies that }$$

$$\begin{bmatrix} I & 0 \\ -D_1^{-1}C_1 & I \end{bmatrix} \begin{bmatrix} (A_1 - B_1D_1^{-1}C_1)^{-1} & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & -B_1 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & D_1^{-1} \end{bmatrix} = X \text{ which is } \begin{bmatrix} A & B \\ C & D \end{bmatrix} \text{ by }$$

definition. Thus $A = (A_1 - B_1 D_1^{-1} C_1)^{-1}$, i.e., A is invertible. Hence we have shown that A is invertible if and only if D_1 is invertible.

$$\begin{split} \text{If } \det(A) \neq 0, \det(X) &= \det \begin{bmatrix} I & -B(D-CA^{-1}B)^{-1} \\ 0 & I \end{bmatrix} \det \begin{bmatrix} I & 0 \\ -CA^{-1} & I \end{bmatrix} \det(X) \\ &= \det \begin{bmatrix} A & 0 \\ 0 & D-CA^{-1}B \end{bmatrix} \\ &= \det(A) \cdot \det(D-CA^{-1}B) \\ &= \det(A) \cdot \det(D_1^{-1}) \quad \text{by (§)} \\ &= \frac{\det(A)}{\det(D_1)}. \end{split}$$

Thus $det(D_1) = \frac{det(A)}{det(X)}$.

Finally, if det(A) = 0, then $det(D_1) = 0 = det(A)/det(X)$; so the theorem is also true when A is singular.

Proof of Theorem 2.1.8. Let M be an $n \times n$ invertible matrix and let $1 \le k < n$. Let $\alpha = \{i_1 < i_2 < \dots < i_k\}$ and $\beta = \{j_1 < j_2 < \dots < j_k\}$ be ordered subsets of $\{1, 2, \dots, n\}$. We need to show that

$$\begin{split} \det M^{\text{-}1}(i_1...i_k|j_1...j_k) &= \frac{(-1)^m}{\det(M)} \det \ M(j_1'...j_{n\cdot k}'|i_1'...i_{n\cdot k}') \\ \text{where } m &= \sum_{r=1}^k (i_r + j_r). \end{split}$$

Define permutation matrices R and P so that X = RMP has $M(\beta'|\alpha')$ as its leading $(n-k) \times (n-k)$ principal submatrix, i.e., $X(n-k) = M(\beta'|\alpha')$. Note that for each $r \in \{1, 2, ..., n-k\}$, R exchanges rows so that row j_r' of M is in row r of X, and P exchanges columns so that column i_r' of M is in column r of X. We may assume that R and P act on M in the following way. Start with M and exchange row j_1' of M with each row above it in turn. This is a total of j_1' - 1 row exchanges. Exchange row j_2' with each row above it except the top row. This is a total of j_2' - 2 row exchanges. Do this for each of rows $j_1', ..., j_{n-k}'$ in order to put rows $j_1', ..., j_{n-k}'$ in positions 1, ..., n-k, respectively.

The total number of row exchanges is $\sum_{r=1}^{n-k} j_r' - \frac{(n-k)(n-k+1)}{2}$. Proceed in a similar way to put columns i_1', \ldots, i_{n-k}' of M in positions $1, \ldots, n-k$, respectively. The total number of column exchanges is $\sum_{r=1}^{n-k} i_r' - \frac{(n-k)(n-k+1)}{2}$. Hence the total number of exchanges is $\delta = \sum_{r=1}^{n-k} (i_r' + j_r') - (n-k)(n-k+1)$. Since (n-k)(n-k+1) is even, δ and $\sum_{r=1}^{n-k} (i_r' + j_r')$ have the same parity. In addition, since $\sum_{r=1}^{k} (i_r + j_r) + \sum_{r=1}^{n-k} (i_r' + j_r') = n(n+1)$ which is even, $\sum_{r=1}^{k} (i_r + j_r)$ and $\sum_{r=1}^{n-k} (i_r' + j_r')$ have the same parity. Letting $m = \sum_{r=1}^{k} (i_r + j_r)$, it follows that $\det(X) = (-1)^{\delta} \cdot \det(M) = (-1)^{m} \cdot \det(M)$.

Since X = RMP, $X^{-1} = P^tM^{-1}R^t$, and for each $r \in \{1, 2, ..., n-k\}$, P^t exchanges rows so that row i_r' of M^{-1} is in row r of X^{-1} , and R^t exchanges columns so that column j_r' of M^{-1} is in column r of X^{-1} . Thus $X^{-1}(n-k) = M^{-1}(\alpha'|\beta')$ which implies that $X^{-1}[k] = M^{-1}(\alpha|\beta)$. By Lemma 2.1.9 and our choice of R and P, we have

$$\det M^{-1}(\alpha|\beta) = \frac{\det M(\beta' \mid \alpha')}{\det(X)}$$

$$= \frac{(-1)^m}{\det(M)} \cdot \det M(\beta' \mid \alpha') \quad \text{by (*)}.$$

We will make use of the following result, which says that in a Hadamard matrix, the determinants of any leading principal submatrix and its complementary trailing principal submatrix are proportional in a special way.

2.1.10 Corollary. [EM] Let H be an $n \times n$ Hadamard matrix and let $1 \le k < n$. Then $|\det H(k)| = n^{k-n/2} |\det H[n-k]|.$

Proof. By Theorem 2.1.8, $|\det H^{-1}(k)| = \frac{|\det H[n-k]|}{|\det(H)|}$. Since $|\det(H)| = n^{n/2}$ and $H^{-1} = (1/n)H^t$, we have $|\det[(1/n)H^t](k)| = n^{-n/2}$ $|\det H[n-k]|$. Also, $\det[(1/n)H^t](k) = (1/n^k)\det H^t(k) = (1/n^k)\det H(k)$. Therefore, we have $(1/n^k)$ $|\det H(k)| = n^{-n/2}$ $|\det H[n-k]|$ which completes the proof.

2.1.11 Corollary. [EM] If H is an $n \times n$ Hadamard matrix which has Property P, and $1 \le k < n$, and H is reduced without row or column exchanges, then

$$p_{n\text{-}k\text{+}1} = n \frac{\left| \det H[k-1] \right|}{\left| \det H[k] \right|}.$$

Proof. By Theorem 2.1.2 and Corollary 2.1.10,

$$p_{n-k+1} = \frac{|\det H(n-k+1)|}{|\det H(n-k)|} = \frac{n^{n-k+1-n/2}|\det H[k-1]|}{n^{n-k-n/2}|\det H[k]|} = n\frac{|\det H[k-1]|}{|\det H[k]|}.$$

2.1.12 Corollary. [EM] Suppose H is an $n \times n$ CP Hadamard matrix, and $1 \le k < n$. If M_{k-1} is any $(k-1) \times (k-1)$ submatrix of the trailing principal submatrix H[k], then $|\det H[k-1]| \ge |\det(M_{k-1})|.$

Proof. Suppose a $(k-1) \times (k-1)$ submatrix M_{k-1} of H[k] satisfied $|\det(M_{k-1})| > |\det H[k-1]|$. We will show that H then cannot be CP. Because $M_{k-1} \neq H[k-1]$, there exist $r, s \ge n-k+1$ and not both n-k+1 such that $M_{k-1} = H(n-k+1...\hat{r}...n|n-k+1...\hat{s}...n)$, where \hat{r} means "omit r." Do the first n-k+1 steps of GECP on H. Then

$$\begin{split} p_{n \cdot k + 1} &= n \frac{\left| \det H[k - 1] \right|}{\left| \det H[k] \right|} & \text{by Corollary 2.1.11} \\ &< n \frac{\left| \det (M_{k - 1}) \right|}{\left| \det H[k] \right|} & \text{by our assumption} \\ &= n \frac{\left| \det H(n - k + 1 \dots \hat{r} \dots n | n - k + 1 \dots \hat{s} \dots n) \right|}{\left| \det H[k] \right|} \\ &= n \frac{\left| \det (H) \cdot \det H^{-1}(1 \dots n - k \text{ sil} \dots n - k \text{ r}) \right|}{\left| \det (H) \cdot \det H^{-1}(n - k) \right|} & \text{by Theorem 2.1.8} \\ &= n \frac{\left| \det \left[(1/n)H^{t} \right](1 \dots n - k \text{ sil} \dots n - k \text{ r}) \right|}{\left| \det \left[(1/n)H^{t} \right](n - k) \right|} & \text{since H is Hadamard} \\ &= \frac{n \frac{1}{n^{n - k + 1}} \left| \det H^{t}(1 \dots n - k \text{ sil} \dots n - k \text{ r}) \right|}{\frac{1}{n^{n - k}} \left| \det H^{t}(n - k) \right|} \\ &= \frac{\left| \det H(1 \dots n - k \text{ sil} \dots n - k \text{ r}) \right|}{\left| \det H(n - k) \right|} \\ &= \frac{\left| \det H(n - k) \right|}{\left| \det H(n - k) \right|} & \text{by Theorem 2.1.2.} \end{split}$$

Hence we have shown that the magnitude of the (n-k+1)st pivot is strictly less than that of the (s, r)-entry of $H^{(n-k)}$ and that (s, r)-entry occurs in $H^{(n-k)}[k]$, thus necessitating row and/or column exchanges in the (n-k+1)st step of GECP on H. Therefore H is not CP, a contradiction. Hence we conclude that $|\det(M_{k-1})| \le |\det H[k-1]|$, and since M_{k-1} was chosen arbitrarily, the proof is complete.

2.1.13 The previous corollary says that |det H[k-1]| is the largest magnitude of a minor of H[k]. This leads to the following:

2.1.14 Corollary. [EM] Suppose H is an $n \times n$ CP Hadamard matrix, and $1 \le k < n$.

Then $\frac{|\det H[k-1]|}{|\det H[k]|}$ is the largest magnitude of an entry of $H[k]^{-1}$.

Proof. By 2.1.3, H(n-k) is invertible. Thus

$$0 \neq |\det H(n-k)| = |\det(H)| |\det H^{-1}[k]|$$
 by Theorem 2.1.8

$$= |\det(H)| |\det [(1/n)H^{t}][k]|$$
 since H is Hadamard

$$= |\det(H)| (1/n^{k}) |\det H^{t}[k]|$$

$$= |\det(H)| (1/n^{k}) |\det H[k]|.$$

Hence det $H[k] \neq 0$, i.e., H[k] is invertible.

By Theorem 2.1.5, $H[k]^{-1} = \frac{1}{\det H[k]} \cdot \operatorname{adj} H[k]$, and by 2.1.13 and the definition of adjugate, $|\det H[k-1]|$ is the largest magnitude of an entry of adj H[k]. Hence $\frac{|\det H[k-1]|}{|\det H[k]|}$ is the largest magnitude of an entry of $H[k]^{-1}$.

Many authors have studied the problem of bounding |det(A)|, where A is a ± 1 matrix. We will make use of a few of these results, which we now state.

2.1.15 Theorem. [Wil] Let d_n denote the largest possible value of the determinant of an $n \times n$ matrix whose entries are ± 1 . The first seven values of the sequence $\langle d_i \rangle$ are 1, 2, 4, 16, 48, 160, 576. For n = 2, ..., 7, if the magnitude of the determinant of an $n \times n$ matrix of ± 1 's is d_n , then the matrix must have a minor whose magnitude is d_{n-1} . This cannot happen when n = 8.

The values of d_1 through d_7 were computed by Williamson in [Wil]. Furthermore, he showed that for n = 2, ..., 7, if A is an $n \times n$ matrix with determinant d_n , then any other

 $n \times n$ matrix with determinant d_n can be obtained from A by a sequence of row exchanges, column exchanges, row negations, and/or column negations. This is also true for n = 8and n = 12 since these matrices are Hadamard, and there is just one equivalence class for 8×8 and 12×12 Hadamards [CW, p. 112].

2.1.16 Examples. For n = 2, ..., 7, an $n \times n$ matrix with determinant d_n is given and a minor is indicated whose magnitude is d_{n-1}.

$$\underline{n=2}$$

$$n = 3$$

$$\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix}, (3, 3) \text{ minor }$$

n = 4

$$n = 5$$

$$\begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \end{bmatrix}, (1, 1) minor$$

n = 6

n = 7

When n = 8, $d_8 = 4096$ and any matrix H whose determinant has magnitude d_8 is Hadamard by Theorem 1.1.7. So $(1/8)H^t = H^{-1} = \pm (1/4096) \cdot adj(H)$ which implies that $adj(H) = \pm 512H^t$. Hence each minor of H has magnitude 512, whereas $d_7 = 576$.

2.2 Pivot Magnitudes

2.2.1 Theorem. [DP] Let $n \ge 4$ and let H be an $n \times n$ Hadamard matrix. Reduce H by GECP. The magnitudes of pivots one through four are 1, 2, 2, and 4, respectively. Proof. Negate rows and columns of H as necessary to make the first row and column positive. Observe that the pivot magnitudes of the resulting matrix H_1 will be the same as those of H. If H_1 is not CP, do the row and column exchanges to H_1 first in the same order they would occur when doing GECP on H_1 . The resulting matrix $H_2 = [h_{ij}]$ is then CP and $H_2^{(n-1)} = H_1^{(n-1)}$; so the pivot magnitudes of H_2 and H will be the same.

The (1, 1)-entry of H_2 is 1 and every entry of the trailing principal submatrix $H_2^{(1)}[n-1]$ is 0 or -2. Thus because H_2 is CP and invertible, $h_{22}^{(1)} = -2$, and it is not hard to see that every entry of $H_2^{(2)}[n-2]$ must be 0 or ± 2 by considering all the possibilities when pivoting on $h_{22}^{(1)}$. Hence $h_{33}^{(2)} = \pm 2$. Each entry of $H_2^{(3)}[n-3]$ is 0, ± 2 , or ± 4 , and we will show $H_2^{(3)}[n-3]$ has an entry with magnitude 4. It then follows that $\left|h_{44}^{(3)}\right| = 4$ since H_2 is CP.

By Theorem 1.1.6, n = 4p for some $p \ge 1$. Each column of H_2 has one of the following four sign patterns in its first three entries:

The mutual orthogonality of the first three rows of H_2 implies that there are exactly p columns of each of the four types. (This follows at once from the argument in the first proof of Theorem 1.1.6.) Because H_2 is CP and invertible, det $H_2(3) \neq 0$ which implies that the first three columns of H_2 must have different sign patterns. Choose any

column $j \ge 4$ of H_2 of the type not represented among columns 1, 2 and 3 of H_2 . There are p of these, so at least one exists. We will show that there exists a row i such that $|\det H_2(1\ 2\ 3\ i|1\ 2\ 3\ j)| = 16$.

By permuting columns 2, 3 and j if necessary, we may assume that H_2 has the pattern (§) in its first three rows and the four columns 1, 2, 3, j. The mutual orthogonality of the first three columns of H_2 implies:

There are exactly p rows of each of types I through IV above. (*)
In particular, there are p rows having pattern +-- in their first three entries, and all these rows lie below the first three rows. At least one of these rows (say, the ith) must have $a_{ij} = +1$. Otherwise, we claim column j of H_2 would have more than 2p negative entries which contradicts its being orthogonal to column 1. To see this, observe that there are eight different patterns that a row of H_2 can have as its 1, 2, 3, j entries:

1	2	3	j	Number of rows with pattern
+	+	+	+	c
+	+	+	-	d
+	-	+	+	e
+	-	+	-	f
+	+	-	+	g
+	+	-	-	h
+	-	-	+	a
+	-	-	-	b

So by (*) we have

$$c+d = e+f = g+h = p.$$
 (1)

Because columns 1 and j are orthogonal, we have

$$c+e+g+a=2p. (2)$$

Similarly, because columns 2 and j are orthogonal,

$$d+e+h+a=2p. (3)$$

And since columns 3 and j are orthogonal,

$$d+f+g+a=2p. (4)$$

Subtract (3) from (2) to get

$$c+g = d+h. (5)$$

Subtract (4) from (2) to get

$$c+e = d+f. (6)$$

Solve for g in (1) and (5) to get c+d-h = g = d+h-c which implies c = h.

Similarly, solve for e in (1) and (6) to get c+d-f=e=d+f-c which implies c=f.

Suppose a = 0, i.e., H_2 has no rows with pattern + - - + in entries 1, 2, 3, j. Then the number of -1's in column j is

$$d+f+h+b = d+c+c+p$$
$$= 2p+c$$

> 2p since $c \ge 1$ because the first row of H_2 is all +1.

This contradicts the fact that column j and column 1 are orthogonal. Hence $a \neq 0$, i.e., there is a row of H_2 (we called it the ith row) with pattern + - - + in entries 1, 2, 3, j.

Thus

By Theorem 2.1.2, $\left|h_{ij}^{(3)}\right| = \frac{\left|\det H_2(1\ 2\ 3\ il1\ 2\ 3\ j)\right|}{\left|\det H_2(3)\right|} = \frac{16}{4} = 4$. Hence because H_2 is CP, $\left|h_{44}^{(3)}\right| = 4$ which completes the proof.

2.2.2 Corollary. [EM] If H is a CP Hadamard matrix whose order is at least 4, then $|\det H(4)| = 16$. Thus by Hadamard's Inequality, H(4) is a Hadamard matrix of order 4.

In [DP], it was shown that the magnitude of the fifth pivot in an 8×8 or larger Hadamard matrix reduced by GECP must be 2 or 3. The following theorem is the key result in [EM] which allows the authors to prove that when H is a 12×12 Hadamard matrix reduced by GECP, the fifth pivot is ± 3 .

2.2.3 Theorem. If H is a 12×12 CP Hadamard matrix, then $|\det H(5)| = 48$.

Proof. Negate rows and columns of H as necessary so that the first row and column of the resulting matrix H_1 are all positive. Observe that H_1 is CP, Hadamard, and $|\det H_1(5)| = |\det H(5)|$. By Corollary 2.2.2, $H_1(4)$ is Hadamard, hence is equivalent to a (3, 1, 0)-symmetric block design by Theorem 1.2.4. Number the objects 1, 2, and 3, and denote block i as B_i . Without loss of generality, we may assume that $B_1' = \{1\}$, $B_2' = \{2\}$, and $B_3' = \{3\}$. This (3, 1, 0)-symmetric block design has incidence matrix

We will now show that some 5×5 submatrix of H_1 with determinant ± 48 has $H_1(4)$ as a submatrix.

By Theorem 1.2.4, H_1 is equivalent to an (11, 5, 2)-symmetric block design. We have already arbitrarily fixed $H_1(4)$. We can enlarge our set of objects to be $\{1, 2, ..., 11\}$. There will be eleven blocks now; call them $B_1, B_2, ..., B_{11}$. The incidence matrix C for $H_1(4)$ is the leading 3×3 principal submatrix of the incidence matrix for H_1 ; hence B_1 is a subset of B_1 , B_2 is a subset of B_2 , and B_3 is a subset of B_3 . From the incidence matrix C, we see that object 3 is not in B_1 or B_2 . Thus without loss of generality, let $B_1 = \{1, 4, 5, 6, 7\}$, and $B_2 = \{2, 4, 5, 8, 9\}$. This chooses 4 and 5 as the pair that appears in B_1 and B_2 , and lets 6, 7, 8, and 9 fill in the remaining spots.

Since there cannot be three blocks containing the same pair, either $B_1 \cap B_2 \cap B_3$ is empty, or it consists of one object which we can call 5 without loss of generality. If $B_1 \cap B_2 \cap B_3 = \{5\}$, then B_3 must contain 6 and 8 so that $|B_1 \cap B_3| = |B_2 \cap B_3| = 2$; hence $B_3 = \{3, 5, 6, 8, 10\}$ or $\{3, 5, 6, 8, 11\}$. If $B_1 \cap B_2 \cap B_3 = \emptyset$, then B_3 must contain 6, 7, 8, and 9 so that $|B_1 \cap B_3| = |B_2 \cap B_3| = 2$; hence $B_3 = \{3, 6, 7, 8, 9\}$.

Let B_4 be a block that contains 1 and 2, but not 3. (There are two blocks that contain any pair such as 1 and 2, and they could not both contain 3 because then there would be too many elements in common.) We claim that B_4 does not contain 4. Suppose, on the contrary, that $4 \in B_4$. Then $5 \notin B_4$ since otherwise 4 and 5 would be in B_1 , B_2 , and B_4 , a contradiction. In addition, neither 6 nor 7 can be in B_4 since that would imply $|B_1 \cap B_4| \ge 3$; and neither 8 nor 9 can be in B_4 since that would imply $|B_2 \cap B_4| \ge 3$. Hence B_4 must contain 10 and 11. Checking the three possibilities for B_3 above shows that in any case, $|B_3 \cap B_4| \le 1$, contrary to the parameters of an (11, 5, 2)-symmetric block design. Thus B_4 contains 1 and 2, but not 3 and not 4.

The information about objects 1 through 4 and blocks B_1 through B_4 tells us that the following is a submatrix of H_1 :

$$M_5 = \begin{bmatrix} H_1(4) & z \\ z^t & -1 \end{bmatrix}$$
, where $z^t = [1 \ 1 \ 1 \ -1]$.

Note that $det(M_5) = 48$. We claim that because H_1 is CP, this implies $|\det H_1(5)| = 48$.

By Theorem 2.1.2,
$$\frac{\left|\det H_1(5)\right|}{\left|\det H_1(4)\right|} = p_5$$
, which, because H_1 is CP, is greater than or equal

to the magnitude of each entry of $H_1^{(4)}[8]$, one of which is $\frac{\left|\det(M_5)\right|}{\left|\det H_1(4)\right|}$ by Theorem 2.1.2.

Thus by Theorem 2.1.15, $48 = d_5 \ge |\det H_1(5)| \ge |\det(M_5)| = 48$. Hence $48 = |\det H_1(5)| = |\det H(5)|$.

2.2.4 Corollary. [EM] If H is a 12×12 CP Hadamard matrix, then

$$p_5 = \frac{|\det H(5)|}{|\det H(4)|} = \frac{48}{16} = 3.$$

2.2.5 Theorem. [EM] If H is a 12 × 12 Hadamard matrix, and H is reduced by GECP, then the absolute values of pivots one through twelve are 1, 2, 2, 4, 3, 10/3, 18/5, 4, 3, 6, 6, and 12, respectively.

Proof. Rearrange rows and columns of H so as to obtain a CP matrix. Call it H. We first show that $|\det H[7]| = 576$. By the preceding corollary, we have $p_5 = 3$. By Corollary 2.1.11, we also have

$$p_5 = p_{12\cdot 8+1} = \frac{12|\det H[7]|}{|\det H[8]|}.$$

Thus $|\det H[7]| = (1/4) |\det H[8]| = (1/4) |\det H[12 - 4]|$ $= (1/4) |12^{6-4}| |\det H(4)|$ by Corollary 2.1.10 $= (1/4) |12^{2}| (16)$ by Corollary 2.2.2 = 576.

By Theorem 2.1.15, this is the largest possible value of the determinant of a 7×7 matrix whose entries are ± 1 . In addition, Theorem 2.1.15 tells us that H[7] must have a minor whose magnitude is 160. Hence $160 \le |\text{det H}[6]|$ since |det H[6]| is greater than or equal to

the magnitude of each minor of H[7] by Corollary 2.1.12. Furthermore, $|\det H[6]| \le d_6 = 160$. Hence $|\det H[6]| = 160$.

In a similar way, we conclude that $|\det H[5]| = 48$, $|\det H[4]| = 16$, $|\det H[3]| = 4$, $|\det H[2]| = 2$, and $|\det H[1]| = 1$. Pivots six through eleven of H now follow from Corollary 2.1.11:

$$p_6 = p_{12-7+1} = \frac{12|\det H[6]|}{|\det H[7]|} = \frac{12 \cdot 160}{576} = \frac{10}{3};$$

$$p_7 = p_{12-6+1} = \frac{12|\det H[5]|}{|\det H[6]|} = \frac{12\cdot 48}{160} = \frac{18}{5};$$

$$p_8 = p_{12-5+1} = \frac{12|\det H[4]|}{|\det H[5]|} = \frac{12\cdot 16}{48} = 4;$$

$$p_9 = p_{12-4+1} = \frac{12|\det H[3]|}{|\det H[4]|} = \frac{12\cdot 4}{16} = 3;$$

$$p_{10} = p_{12-3+1} = \frac{12|\det H[2]|}{|\det H[3]|} = \frac{12\cdot 2}{4} = 6;$$

$$p_{11} = p_{12\cdot 2+1} = \frac{12|\det H[1]|}{|\det H[2]|} = \frac{12\cdot 1}{2} = 6.$$

And $p_{12} = 12$ by Corollary 2.1.7.

PART TWO

COMPLETION OF PARTIAL POSITIVE DEFINITE MATRICES

CHAPTER 1

BACKGROUND

Henceforth all matrices are assumed to be $n \times n$ unless otherwise indicated.

1.1 Positive Definite Matrices

- 1.1.1 <u>Definitions</u>. The Hermitian adjoint A^* (also called conjugate transpose) of a complex matrix A is defined by $A^* = \overline{A}^t$, where \overline{A} is the component-wise conjugate of A. A complex matrix A is called Hermitian if $A^* = A$. The set of all $n \times n$ Hermitian matrices will be denoted H.
- **1.1.2** <u>Definition</u>. A Hermitian matrix A is positive definite if $x^*Ax > 0$ for all nonzero $x \in \mathbb{C}^n$. If the above inequality is changed to $x^*Ax \ge 0$ for all nonzero $x \in \mathbb{C}^n$, then A is said to be positive semidefinite.
- 1.1.3 Remark. For an $n \times n$ Hermitian matrix A, there exists a unitary matrix U such that U^*AU is a real diagonal matrix. In other words, the eigenvalues of A are real and there is a set of n orthonormal eigenvectors for A.

- **1.1.4** Theorem. [HJ, 7.2.1] A Hermitian matrix A is positive definite (semidefinite) if and only if all of its eigenvalues are positive (nonnegative).
- Proof. (\Rightarrow) Let A be positive definite and λ be an eigenvalue of A with associated eigenvector x. Then $x^*Ax = x^*\lambda x = \lambda x^*x$. Thus $\lambda = \frac{x^*Ax}{x^*x}$ is positive since it is a ratio of two positive numbers.
 - (\Leftarrow) If each eigenvalue of A is positive, then for any nonzero $x \in \mathbb{C}^n$, we have $x^*Ax = x^*U^*DUx \quad \text{where } D = \operatorname{diag}(\lambda_1, \lambda_2, ..., \lambda_n) \text{ is the diagonal matrix of eigenvalues of A and U is unitary}$

$$= y^*Dy \qquad \text{where } y = Ux$$

$$= \sum_{i=1}^{n} \lambda_i \overline{y_i} y_i \qquad \text{where } y^* = \left[\overline{y_1} ... \overline{y_n} \right]$$

$$= \sum_{i=1}^{n} \lambda_i |y_i|^2$$

$$> 0.$$

The positive semidefinite case is proved similarly.

- 1.1.5 Remark. Since the trace of A is the sum of its eigenvalues and the determinant of A is the product of its eigenvalues, it follows from the above theorem that $\det(A) > 0$ and $\operatorname{tr}(A) > 0$ for positive definite A, and $\det(A) \ge 0$ and $\operatorname{tr}(A) \ge 0$ for positive semidefinite A.
- **1.1.6** For a Hermitian matrix $H = [h_{rs}]$, $h_{rs} = \overline{h_{sr}}$ and thus h_{rr} is real. In order to understand the optimization theorems in [GJSW], it is helpful to identify H with an element of \mathbb{R}^{n^2} as follows: for $1 \le r \le s \le n$, let $h_{rr} \equiv x_{rr}$, and for r < s, let $h_{rs} \equiv x_{rs} + iy_{rs}$, where x_{rs} and y_{rs} are real. Create the n^2 -tuple of all x_{rs} , y_{rs} by lexicographic ordering:

$$[x_{11}, x_{12}, y_{12}, x_{13}, y_{13}, ..., x_{1n}, y_{1n}, x_{22}, x_{23}, y_{23}, ..., x_{2n}, y_{2n}, ..., x_{nn}].$$

Observe that this defines an isomorphism from the set of $n \times n$ Hermitian matrices H onto \mathbb{R}^{n^2} (both real vector spaces) and the identification provides a topology for H.

We will use the terms "open set," "closed set," "interior," "closure," "boundary," and "limit point" as defined in the usual topology on R^{n^2} [Pat].

1.1.7 Definition. Given a matrix A, A(k) will denote the leading $k \times k$ principal submatrix of A.

1.1.8 Theorem. Let A be $n \times n$ Hermitian. Then the following are equivalent.

- (1) A is positive definite.
- (2) A(k) is positive definite for each k = 1, ..., n.
- (3) $\det A(k) > 0$ for each k = 1, ..., n.
- (4) There exist a lower triangular L with diagonal entries 1 and a real diagonal D with positive diagonal entries such that A = LDL*.

Proof. (1) \Rightarrow (2) Let $k \in \{1,...,n\}$ and let x be a nonzero k-tuple. Define an n-tuple $y = [x \ 0]^t$. Then $y \neq \theta$, where θ denotes the zero vector; so $y^*Ay > 0$. In addition, $x^*A(k)x = y^*Ay$; thus A(k) is positive definite.

- $(2) \Rightarrow (3)$ is immediate since the determinant of a matrix is the product of its eigenvalues, each of which is positive when the matrix is positive definite.
- (3) \Rightarrow (4) Since a_{11} = det A(1) > 0, the first step of Gaussian elimination can be performed without row exchanges obtaining

$$A^{(1)} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a'_{22} & \cdots & a'_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a'_{n2} & \cdots & a'_{nn} \end{bmatrix}.$$

Since adding a multiple of one row to another does not affect the determinant, we have

det A(2) = det A⁽¹⁾(2) = $a_{11}a'_{22}$. Since det A(2) > 0 by hypothesis and a_{11} > 0 from above, a'_{22} > 0. Thus the next step of Gaussian elimination can be performed without row exchanges obtaining

$$A^{(2)} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & 0 & a'_{33} & \cdots & a'_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a'_{n3} & \cdots & a'_{nn} \end{bmatrix}, \text{ where } a'_{33} > 0 \text{ by the same reasoning as before.}$$

Continuing in this way, we reduce A to an upper triangular matrix U_1 with positive diagonal entries.

Notice that

$$A^{(1)} = L_1 A, \text{ where } L_1 = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -m_{21} & 1 & 0 & \cdots & 0 \\ -m_{31} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -m_{n1} & 0 & 0 & \cdots & 1 \end{bmatrix} \text{ with } m_{k1} = a_{k1}/a_{11}, \text{ and }$$

$$A^{(2)} = L_2 A^{(1)} = L_2 L_1 A, \text{ where } L_2 = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & -m_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -m_{n2} & 0 & \cdots & 1 \end{bmatrix} \text{ with } m_{k2} = a'_{k2} / a'_{22}.$$

This pattern continues for each $A^{(k)}$ through k = n - 1. Hence we can write

$$U_1 = L_{n-1} \cdots L_1 A$$
.

Then

$$A = L_1^{-1}L_2^{-1}\cdots L_{n-1}^{-1}U_1$$
 and

$$L_{1}^{-1}L_{2}^{-1}\cdots L_{n-1}^{-1} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ m_{21} & 1 & 0 & \cdots & 0 \\ m_{31} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ m_{n1} & 0 & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & m_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & m_{n2} & 0 & \cdots & 1 \end{bmatrix} \cdots L_{n-1}^{-1}$$

$$= \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ m_{21} & 1 & 0 & \cdots & 0 \\ m_{31} & m_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ m_{n1} & m_{n2} & m_{n3} & \cdots & 1 \end{bmatrix} = L.$$

Now let D be the diagonal matrix of main diagonal entries of U_1 and let $U = D^{-1}U_1$. Then A = LDU, where L and U are lower and upper triangular, respectively, and have diagonal entries 1.

Since $A = A^*$ and D is real, $LDU = U^*DL^*$. Hence $D^{-1}(U^*)^{-1}LD = L^*U^{-1}$. The left side is lower triangular and the right side is upper triangular; thus both must be diagonal. Since L^* and U^{-1} are upper triangular with diagonal entries 1, their product must have diagonal entries 1; hence $L^*U^{-1} = I$ which means $L^* = U$. Thus $A = LDL^*$ as claimed. (4) \Rightarrow (1) Let x be nonzero in C^n and let $y = L^*x$. Then $x^*Ax = y^*Dy = \sum_{i=1}^n d_i |y_i|^2 > 0$, where $D = \operatorname{diag}(d_1, \ldots, d_n)$ and $y^* = [\overline{y_1} \ldots \overline{y_n}]$. Hence A is positive definite.

Notice that with appropriate generalizing, the $(1) \Rightarrow (2)$ part of the above proof can be used to prove the following:

1.1.9 Theorem. [HJ, 7.1.2] Every principal submatrix of a positive (semi)definite matrix is positive (semi)definite.

1.1.10 Since det(A) is a polynomial in the entries of A, the function det: $\mathbf{H} \to \mathbf{R}$ is continuous. For each k = 1, ..., n, we define $V_k \equiv \{A \in \mathbf{H}: \det A(k) > 0\}$. Since $(0, \infty)$ is an open set in \mathbf{R} and det is continuous, V_k must be open in \mathbf{H} for each k = 1, ..., n. Hence $\bigcap_{i=1}^n V_i$ is open in \mathbf{H} since it is the intersection of a finite number of open sets in \mathbf{H} . We define $S_0 \equiv \bigcap_{i=1}^n V_i$ which equals $\{A \in \mathbf{H}: A \text{ is positive definite}\}$ by Theorem 1.1.8. Thus S_0 , the set of positive definite $n \times n$ Hermitian matrices, is open in \mathbf{H} .

The following result justifies some claims made in [GJSW].

1.1.11 Theorem. The closure of S_0 , which we will call S, is the set of all positive semidefinite $n \times n$ matrices. Furthermore, S_0 is the interior of S.

Proof. Since $S = \overline{S_0}$, if $A \in S$, then either $A \in S_0$ or A is a limit point of S_0 . In either case, there exists a sequence $\langle A_i \rangle$ in S_0 such that $\lim_{i \to \infty} A_i = A$, i.e., $\lim_{i \to \infty} (A_i)_{rs} = A_{rs}$, where $(A_i)_{rs}$ denotes the (r, s)-entry of A_i . If x is a nonzero vector in \mathbf{C}^n , $x^*A_i x > 0$ for each i. Furthermore, since addition, multiplication, and conjugation are continuous functions, we have $\lim_{i \to \infty} x^*A_i x = x^*Ax$. Hence $x^*Ax \ge 0$, i.e., A is positive semidefinite.

Conversely, suppose A is positive semidefinite. Let $\varepsilon > 0$. Then by Theorem 1.1.4, $A + \varepsilon I$ is positive definite since each eigenvalue of $A + \varepsilon I$ is of the form $\lambda + \varepsilon$ where λ is an eigenvalue of A. Since $\lim_{\varepsilon \to 0} (A + \varepsilon I) = A$, A is in the closure of S_0 .

To see that S_0 is the interior of S, first recall that S_0 is open in H. Hence $S_0 \subseteq S^o$, where S^o denotes the interior of S. To show that $S^o \subseteq S_0$, we will prove that if $A \notin S_0$, then $A \notin S^o$. Let $A \in S - S_0$. Then A is positive semidefinite, but not positive definite. Hence its smallest eigenvalue is zero. Let $\varepsilon > 0$ and note that the smallest eigenvalue of $A - \varepsilon I$ is $-\varepsilon$. Thus $A - \varepsilon I \notin S$. Since $\lim_{\varepsilon \to 0} (A - \varepsilon I) = A$, we conclude that no neighborhood of A is inside S. Hence $A \notin S^o$, as desired.

Henceforth we will write S^{o} for the set of positive definite $n\times n$ matrices.

1.1.12 It is easy to verify that S is a cone [HJ, 7.1.3]: that is, if a, $b \ge 0$ and M, $N \in S$, then $aM + bN \in S$.

1.2 Partial Matrices and Graphs

- **1.2.1** <u>Definitions.</u> A partial matrix is a matrix that has at least one unspecified, or free, entry. A partial Hermitian matrix A is a partial matrix with the property that if a_{rs} is specified, then a_{sr} is specified and $a_{sr} = \overline{a_{rs}}$.
- **1.2.2** <u>Definitions.</u> A completion of a partial matrix $A = [a_{kp}]$ is a matrix $M = [m_{kp}]$ with all entries specified and which satisfies $m_{rs} = a_{rs}$ for each specified entry a_{rs} in A. A Hermitian completion of a partial Hermitian matrix is a completion that is Hermitian. A positive (semi)definite completion of a partial Hermitian matrix is a completion that is Hermitian and positive (semi)definite.
- **1.2.3** <u>Definitions.</u> A finite undirected graph G = (V, E) is a finite set of vertices V together with a set of edges E which is a subset of $\{\{x, y\}: x, y \in V\}$. G may contain loops, i.e., x may equal y for an edge $\{x, y\} \in E$. Unless otherwise indicated, we assume that $V = \{1, 2, ..., n\}$.
- **1.2.4 Definition.** A clique is a subset $C \subseteq V$ having the property that $\{x, y\} \in E$ for all $x, y \in C$, including all loops $\{x, x\}$ for $x \in C$.

It is not customary in graph theory to include all loops in the definition of clique as we have done, but it is important to have them here. In addition, many graph theory texts define a clique as a subgraph rather than a subset of vertices as we have done. Our definition allows us to develop important concepts in chapter four.

- **1.2.5** <u>Definitions</u>. Given a graph G = (V, E), a *G-partial matrix* $A(G) = [a_{rs}]$ is a partial matrix whose (r, s)-entry is specified if and only if $\{r, s\} \in E$. (So either a_{rs} and a_{sr} are both specified or neither is specified, because G is undirected.) We say that A(G) is *G-partial positive (semi)definite* if A(G) is partial Hermitian and for any clique C of G, the principal submatrix $[a_{kp}]$ of A(G), $k, p \in C$, is positive (semi)definite. In other words, a G-partial Hermitian matrix A(G) is G-partial positive (semi)definite if every completely specified principal submatrix of A(G) is positive (semi)definite.
- **1.2.6** Given a graph G = (V, E) and $A(G) = [a_{kp}]$ a particular G-partial matrix, we define $\mathbf{H}(A(G))$ to be the set of all Hermitian completions of A(G). For each $\{r, s\} \notin E$ and $r \neq s$, $a_{rs} = x_{rs} + iy_{rs}$ determines two real variables, x_{rs} and y_{rs} . Notice that a_{sr} determines the same two real variables since $a_{sr} = \overline{a_{rs}}$. For each $\{r, r\} \notin E$, $a_{rr} = x_{rr}$ determines one real variable, x_{rr} . If m is the number of real variables in A(G) determined by all pairs $\{r, s\} \notin E$, then $\mathbf{H}(A(G))$ can be identified with $\mathbf{R}^{\mathbf{m}}$ in the same way we identified H with $\mathbf{R}^{\mathbf{n}^2}$ in 1.1.6. Hence $\mathbf{H}(A(G))$ is closed in H because an m-dimensional subspace of $\mathbf{R}^{\mathbf{n}^2}$ is closed in $\mathbf{R}^{\mathbf{n}^2}$. Define $S(A(G)) \equiv S \cap \mathbf{H}(A(G))$ which is the set of all positive semidefinite completions of A(G). Then S(A(G)) is closed in H since it is the intersection of two closed subsets of H.

The set of all positive definite completions of A(G) is $S^o \cap H(A(G))$ which is open in H(A(G)) since S^o is open in H.

The following theorem justifies claims in [GJSW].

1.2.7 Theorem. Suppose there exists a positive definite completion of A(G). Then $S^o \cap \mathbf{H}(A(G)) \neq \emptyset$ and its closure is S(A(G)). Furthermore, $S^o \cap \mathbf{H}(A(G))$ is the interior of S(A(G)) relative to $\mathbf{H}(A(G))$.

Proof. Let B be a positive definite completion of A(G). Then $B \in S^o \cap \mathbf{H}(A(G))$. Since the closure of $S^o \cap \mathbf{H}(A(G))$ is a subset of $\overline{S^o} \cap \overline{\mathbf{H}(A(G))}$ which equals $S \cap \mathbf{H}(A(G))$, we have $\overline{S^o \cap \mathbf{H}(A(G))} \subseteq S(A(G))$.

Let $C \in S(A(G))$ and $t \in (0, 1)$. Then (1 - t)B + tC is a Hermitian completion of A(G). Moreover (1 - t)B + tC is positive definite: if $x \neq 0$, $x^*[(1 - t)B + tC]x = (1 - t)x^*Bx + tx^*Cx > 0$ because $x^*Bx > 0$, 1 - t > 0, and $x^*Cx \ge 0$. Hence $(1 - t)B + tC \in S^0 \cap H(A(G))$. As t approaches 1, (1 - t)B + tC approaches C. Thus C is a limit point of $C \cap H(A(G))$ which implies $C \in C \cap H(A(G))$. Since C was chosen arbitrarily, C and C arbitrarily, C and C arbitrarily, C approaches C arbitrarily, C approaches C arbitrarily, C approaches C arbitrarily, C and C arbitrarily, C arbitrarily arb

To see that $S^o \cap \mathbf{H}(A(G))$ is the interior of S(A(G)) relative to $\mathbf{H}(A(G))$, first recall that $S^o \cap \mathbf{H}(A(G))$ is open in $\mathbf{H}(A(G))$. Thus $S^o \cap \mathbf{H}(A(G)) \subseteq S^o(A(G))$ where $S^o(A(G))$ denotes the interior of S(A(G)) relative to $\mathbf{H}(A(G))$.

Let $W \in S^o(A(G))$. We need to show that W must be positive definite. Let B be a positive definite completion of A(G). Since W is in the interior of S(A(G)) relative to H(A(G)), there is a subset U of S(A(G)), open in H(A(G)), such that $W \in U$. Since the whole line $\{tW + (1 - t)B: t \in R\}$ is in H(A(G)), and U is open in H(A(G)) and contains W, there exists an $\varepsilon > 0$ such that $W_0 = (1 + \varepsilon)W + (-\varepsilon)B$ is also in U. Thus $W_0 \in S^o(A(G))$ which implies W_0 is positive semidefinite. By the reasoning in the first part of this proof, $tW_0 + (1 - t)B$ is positive definite for each $t \in (0, 1)$. Let $t_0 = \frac{1}{1 + \varepsilon}$. Then $t_0W_0 + (1 - t_0)B \equiv W$; so W is positive definite, as desired. Since W was chosen arbitrarily, $S^o(A(G)) \subseteq S^o \cap H(A(G))$. Thus we have shown $S^o(A(G)) = S^o \cap H(A(G))$.

Henceforth we will write $S^o(A(G))$ for the set of all positive definite completions of A(G).

CHAPTER 2

CONVEX SETS AND STRICTLY CONCAVE FUNCTIONS

2.1 Introduction

2.1.1 The purpose of this chapter is to lay the groundwork for chapter 3 where we will consider the following cases given a graph G and a particular G-partial matrix A(G).

(Case 1) The graph G contains a loop at every vertex, i.e., every diagonal entry of A(G) is specified. Then S(A(G)) is compact, and we will see that the determinant function takes its maximum on S(A(G)) at a unique $B \in S^{o}(A(G))$.

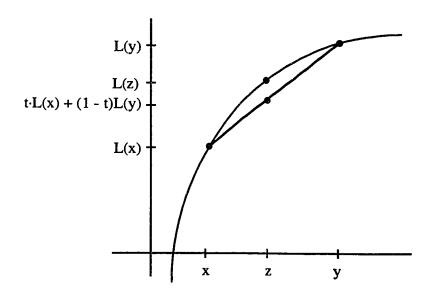
(Case 2) Some loop is missing in G. That is, some diagonal entry is unspecified in A(G). Then S(A(G)) is closed but not compact, and the determinant function is not bounded on S(A(G)). In this case, we will study the behavior of the determinant on compact subsets of S(A(G)) such as $K = \{Z \in S(A(G)): tr(Z) \le T\}$ where $0 < T < \infty$. We will show that the determinant function takes its maximum on such K at a unique B, but this time B is on the boundary of K.

2.1.2 Definition. A subset K of \mathbb{R}^n is *convex* if the line segment joining any two points in K lies entirely in K. That is, if for every $x, y \in K$ and $t \in (0, 1)$, $tx + (1 - t)y \in K$, then K is *convex*.

2.1.3 <u>Definition</u>. If K is a convex subset of \mathbb{R}^n , a function $f: K \to \mathbb{R}$ will be called *strictly concave* if f(tx + (1 - t)y) > tf(x) + (1 - t)f(y) for every distinct pair x, y in K and each $t \in (0, 1)$.

2.1.4 For $x, y \in K$ and fixed t between 0 and 1, tx + (1 - t)y is a point on the segment joining x and y. In addition, (tx + (1 - t)y, tf(x) + (1 - t)f(y)) is a point on the segment joining (x, f(x)) and (y, f(y)).

2.1.5 Observe that the function $L(x) = \log(x)$ is strictly concave on $(0, \infty)$: Let z = tx + (1 - t)y.



2.2 Properties of the Determinant Function; Convex Optimization

The following is somewhat stronger than 7.2.7 in [HJ].

2.2.1 Lemma. A is positive definite if and only if there exists a positive definite matrix C such that $A = C^*C$.

Proof. Suppose A is positive definite. Then A can be unitarily diagonalized as $A = UDU^*$, where $D = diag(\lambda_1, ..., \lambda_n)$ is the diagonal matrix of eigenvalues of A (all positive) and U is unitary. We define $C = UD^{1/2}U^*$, where $D^{1/2} = diag(\lambda_1^{1/2}, ..., \lambda_n^{1/2})$, and $\lambda_i^{1/2}$ denotes the unique positive square root of λ_i , for each i. Since $C = C^*$ and each eigenvalue $\lambda_i^{1/2}$ of C is positive, C is positive definite. Moreover,

$$C^*C = C^2 = UD^{1/2}U^*UD^{1/2}U^* = UDU^* = A$$
.

Conversely, suppose $A = C^*C$ where C is positive definite. Then $A^* = A$ and since det(C) > 0, C is invertible. So if $x \ne 0$, $Cx \ne 0$ and we have

$$x^*Ax = x^*C^*Cx = (Cx)^*Cx > 0.$$

The following is much like 7.6.5 in [HJ], but somewhat more specific.

2.2.2 Lemma. Suppose A and B are positive definite. Then there exists a nonsingular matrix P such that P^*AP and P^*BP are both diagonal and det(P) = 1.

Proof. By the previous lemma, there exists a positive definite C such that $A = C^*C = C^*IC$. Then $I = (C^*)^{-1}AC^{-1} = (C^{-1})^*AC^{-1}$. Now $(C^{-1})^*BC^{-1}$ is Hermitian so it can be unitarily diagonalized. Let U be unitary such that $U(C^{-1})^*BC^{-1}U^*$ is diagonal, and let $Q = C^{-1}U^*$. Then $Q^*BQ = U(C^{-1})^*BC^{-1}U^*$ and

$$Q^*AQ = U(C^{-1})^*AC^{-1}U^* = UIU^*$$
 from above

= I since U is unitary.

Hence Q^*BQ and Q^*AQ are both diagonal. Letting P = (1/d)Q, where $d^n = \det(Q)$, we have $\det(P) = \frac{1}{d^n} \det(Q) = 1$, and P^*AP and P^*BP are diagonal.

2.2.3 Theorem. [GJSW] The function f(Z) = logdet(Z) is strictly concave on S^o. That is, for positive definite A and B, and 0 < t < 1,

$$logdet[tA + (1 - t)B] > t \cdot logdet(A) + (1 - t)logdet(B).$$

Proof. Let A, B \in So. By Lemma 2.2.2, there exists a nonsingular P such that $P^*AP = D$ = diag(d₁₁,..., d_{nn}) and $P^*BP = C = \text{diag}(c_{11},...,c_{nn})$ and det(P) = 1. Then for any $t \in (0, 1)$, we have

$$\begin{aligned} \log \det \left[tA + (1-t)B \right] &= \operatorname{logdet} \left(P^*[tA + (1-t)B]P \right) & \operatorname{because} \det(P) = 1 \\ &= \operatorname{logdet} \left[tD + (1-t)C \right] \\ &= \operatorname{log} \prod_{i=1}^n \left(td_{ii} + (1-t)c_{ii} \right) \\ &= \sum_{i=1}^n \operatorname{log} \left(td_{ii} + (1-t)c_{ii} \right) \\ &> \sum_{i=1}^n \left(t \operatorname{log} d_{ii} + (1-t)\operatorname{log} c_{ii} \right) & \operatorname{by the strict concavity of log}(x) \\ &= t \sum_{i=1}^n \operatorname{log} d_{ii} + (1-t) \sum_{i=1}^n \operatorname{log} c_{ii} \\ &= t \cdot \operatorname{logdet}(D) + (1-t)\operatorname{logdet}(C) \\ &= t \cdot \operatorname{logdet}(A) + (1-t)\operatorname{logdet}(B) & \operatorname{since} \det(P) = 1. \end{aligned}$$

2.2.4 Henceforth, Z(k | p) will denote the (k, p)-minor of Z, i.e., the determinant of the submatrix obtained by omitting row k and column p of Z. This is the notation used in [GJSW] and it works well. (The observant reader may recall that Z(klp) meant something different in part one of this paper.)

2.2.5 <u>Theorem.</u> [GJSW] Suppose Z is partial Hermitian, and for each free entry z_{kp} , $z_{pk} = \overline{z_{kp}}$ and we set $z_{kp} = x_{kp} + iy_{kp}$ as in 1.2.6, where x_{kp} and y_{kp} are real variables. Let

 $Z(k \mid p)$ denote the (k, p)-minor of Z. Then

$$\frac{\partial}{\partial x_{kk}} \det(Z) = Z(k \mid k),$$

and if $k \neq p$,

$$\frac{\partial}{\partial x_{kp}} \det(Z) = 2(-1)^{k+p} \operatorname{Re}(Z(k \mid p))$$
 and

$$\frac{\partial}{\partial y_{kp}} \det(Z) = -2(-1)^{k+p} \operatorname{Im}(Z(k \mid p)),$$

where Re and Im denote real and imaginary parts, respectively.

Proof. Observe that when k = p, $x_{kk} = z_{kk}$. Thus

$$\frac{\partial}{\partial x_{kk}} \det(Z) = \frac{\partial}{\partial z_{kk}} \det(Z)$$

$$= \frac{\partial}{\partial z_{kk}} \sum_{j=1}^{n} z_{kj} (-1)^{k+j} (Z(k \mid j)) \qquad \text{[expanding det(Z) about row k]}$$

$$= (-1)^{k+k} (Z(k \mid k)) \quad \text{since } \frac{\partial z_{kj}}{\partial z_{kk}} = 1 \text{ when } j = k \text{ and equals 0 otherwise}$$

$$= Z(k \mid k).$$

Now let $k \neq p$. Then x_{kp} and y_{kp} appear only in z_{kp} and z_{pk} which is $\overline{z_{kp}}$. Using the

Chain Rule [BL, 4.4], we get

$$\frac{\partial}{\partial x_{kp}} \text{det}(Z) = \sum_{r,s=1}^n \frac{\partial}{\partial z_{rs}} \text{det}(Z) \cdot \frac{\partial z_{rs}}{\partial x_{kp}}.$$

Observe that $\frac{\partial z_{kp}}{\partial x_{kp}} = \frac{\partial z_{pk}}{\partial x_{kp}} = 1$ and all other $\frac{\partial z_{rs}}{\partial x_{kp}} = 0$. Thus the above sum becomes

 $\frac{\partial}{\partial z_{kp}} \det(Z) + \frac{\partial}{\partial z_{pk}} \det(Z)$. Expanding $\det(Z)$ about row k in the first summand and about

row p in the second, we get

$$\begin{split} \frac{\partial}{\partial z_{kp}} \det(Z) + \frac{\partial}{\partial z_{pk}} \det(Z) &= \frac{\partial}{\partial z_{kp}} \sum_{j=1}^{n} z_{kj} (-1)^{k+j} (Z(k \mid j)) + \frac{\partial}{\partial z_{pk}} \sum_{j=1}^{n} z_{pj} (-1)^{p+j} (Z(p \mid j)) \\ &= (-1)^{k+p} (Z(k \mid p)) + (-1)^{p+k} (Z(p \mid k)) \\ &= (-1)^{k+p} [Z(k \mid p) + Z^*(p \mid k)] \quad \text{since } Z \text{ is Hermitian} \\ &= (-1)^{k+p} [Z(k \mid p) + \overline{Z^t(p \mid k)}] \\ &= (-1)^{k+p} [Z(k \mid p) + \overline{Z^t(k \mid p)}] \\ &= 2 (-1)^{k+p} Re(Z(k \mid p)). \end{split}$$

Now differentiating with respect to y_{kp} (using the Chain Rule again), we get

$$\frac{\partial}{\partial y_{kp}} \det(Z) = \sum_{r,s=1}^{n} \frac{\partial}{\partial z_{rs}} \det(Z) \cdot \frac{\partial z_{rs}}{\partial y_{kp}}.$$

Observe that $\frac{\partial z_{kp}}{\partial y_{kp}} = i$, $\frac{\partial z_{pk}}{\partial y_{kp}} = -i$, and all other $\frac{\partial z_{rs}}{\partial y_{kp}} = 0$. Proceeding as before, the above

sum equals

$$\frac{\partial}{\partial z_{kp}} \det(Z) \cdot i + \frac{\partial}{\partial z_{pk}} \det(Z) \cdot (-i) = (-1)^{k+p} (Z(k \mid p)) \cdot i + (-1)^{p+k} (Z(p \mid k)) \cdot (-i)$$

$$= i(-1)^{k+p} [Z(k \mid p) - Z(p \mid k)]$$

$$= i(-1)^{k+p} [Z(k \mid p) - \overline{Z(k \mid p)}]$$

$$= i(-1)^{k+p} \cdot 2 \operatorname{Im}(Z(k \mid p)) \cdot i$$

$$= -2(-1)^{k+p} \operatorname{Im}(Z(k \mid p)).$$

The following theorem is stated in [GJSW] and said to be well-known. Not finding it explicitly stated in standard references, we include a proof.

- **2.2.6** Theorem. Let $g: U \to \mathbb{R}$ be a continuous function defined on an open subset U of \mathbb{R}^n and let $K \subset U$ be such that
 - (1) K is convex, compact, and |K| > 1 (i.e., K has more than one element), and
 - (2) $g(x) \ge 0$ for all x in K, and g is strictly log-concave on K (that is, log(g(x)) is strictly concave on K where we agree that $log(0) = -\infty$).

Then the following are true:

- (i) There exists a unique b ∈ K such thatg(b) = max{g(x): x ∈ K}.
- (ii) If g is continuously differentiable, this maximizing point b is the unique element ofK satisfying g(b) > 0 and

$$\langle \nabla g(b), x - b \rangle \le 0$$
 for all $x \in K$,

where ∇g denotes the gradient of g and $\langle \ , \ \rangle$ is the standard inner product on \mathbb{R}^n . Proof of (i). Since K is compact and g is continuous on K, there exists $b \in K$ such that $g(b) = \max\{g(x): x \in K\}$. Suppose there exists $b_1 \neq b$ such that $g(b_1) = g(b)$. Then because $\log(g(x))$ is strictly concave on K, we have

$$\log(g(\frac{1}{2}b_1 + \frac{1}{2}b)) > \frac{1}{2}\log(g(b_1)) + \frac{1}{2}\log(g(b)) = \log(g(b)).$$

This is a contradiction to the maximality of g(b) since $\frac{1}{2}b_1 + \frac{1}{2}b \in K$ because K is convex, and the log function is strictly increasing. Thus b is the unique element of K where $\max\{g(x): x \in K\}$ occurs.

Proof of (ii). Since |K| > 1 and g assumes its maximum only once, g is not constant; also $g(x) \ge 0$ on K, so g(b) > 0.

Let $x \in K$. Then the segment joining x and b lies entirely in K since K is convex. Hence by the Mean-Value Theorem [BL, 3.9.1], for every $y \neq b$ on the segment, there exists c between y and b such that

$$g(y) - g(b) = \langle \nabla g(c), y - b \rangle.$$

Since g(y) - g(b) < 0 by (i) and x - b is a positive scalar multiple of y - b, we have $\langle \nabla g(c), x - b \rangle < 0$ as $c \to b$. Since g is continuously differentiable (i.e., ∇g is continuous), $\langle \nabla g(b), x - b \rangle \leq 0$. Hence we have shown that the maximizing point b satisfies g(b) > 0 and $\langle \nabla g(b), x - b \rangle \leq 0$ for all $x \in K$. We need only show that b is the unique element of K satisfying these properties.

Let $a \in K$, g(a) > 0, and $a \ne b$. Then g(a) < g(b). We want to show there exists $z \in K$ such that $\langle \nabla g(a), z - a \rangle > 0$. (In fact, z = b will work.) We claim that g is strictly increasing as you move toward b along the segment joining a and b. For otherwise, since the log function is strictly increasing, log(g(x)) fails to be strictly concave which is a contradiction. Letting $h = \frac{b-a}{\|b-a\|}$, we then have that the directional derivative $\frac{\partial g}{\partial h}(a) \ge 0$. Since $\frac{\partial g}{\partial h}(a) = \langle \nabla g(a), h \rangle$ [BL, 3.8.6(ii)], it follows that $\langle \nabla g(a), b - a \rangle \ge 0$. It just remains to prove that, in fact, $\langle \nabla g(a), b - a \rangle > 0$. To do this, we show that $\frac{\partial g}{\partial h}(a) > 0$ which is an immediate consequence of the following:

Lemma. Let $0 in <math>\mathbb{R}$, $g: (p, q) \to \mathbb{R}$ be differentiable, and g(x) > 0 for each $x \in (p, q)$. Also suppose g is strictly log-concave and strictly increasing from p to q. Then g'(x) > 0 for every $x \in (p, q)$.

Proof. Define $G(x) = \log(g(x))$, so $G'(x) = \frac{1}{g(x)}g'(x)$. Since g is strictly increasing from p to q, and the logarithmic function is strictly increasing, G is strictly increasing from p to

q. Fix x in (p, q) and y in (x, q) so that p < x < y < q. Let s be the slope of the line L through (x, G(x)) and (y, G(y)). Then $s = \frac{G(y) - G(x)}{y - x} > 0$ since G is strictly increasing

from p to q. Let x < d < y. Then g(x) < g(d) < g(y) since g is strictly increasing from p to q. Let $t \in (0, 1)$ such that g(d) = t(g(x)) + (1 - t)(g(y)). The strict log-concavity of g implies that $\log(g(d)) = \log[t(g(x)) + (1 - t)(g(y))] > t \cdot \log(g(x)) + (1 - t)\log(g(y))$, i.e., G(d) > tG(x) + (1 - t)G(y) which means (d, G(d)) lies above L. Thus

$$\frac{G(d)-G(x)}{d-x}>s \text{ for each } d\in (x,q) \text{ which implies } G'(x)=\lim_{d\to x}\frac{G(d)-G(x)}{d-x}\geq s>0.$$

Since x was chosen arbitrarily and g(x) > 0, we have g'(x) = g(x)G'(x) > 0 for each $x \in (p, q)$.

2.3 Convex Hulls and Compactness

The following basic theory about convex sets is important here so we include the proofs.

- **2.3.1** <u>Definition</u>. For fixed $m \in \mathbb{N}$ and i = 1, ..., m, let λ_i be a nonnegative real number, and suppose $\lambda_1 + \lambda_2 + \cdots + \lambda_m = 1$. Then $\lambda_1 x_1 + \lambda_2 x_2 + \cdots + \lambda_m x_m$ is called a *convex combination* of the points $x_1, ..., x_m$.
- 2.3.2 <u>Lemma</u>. [Lay, 2.15] A subset K of Rⁿ is convex if and only if every convex combination of points of K lies in K.

Proof. (⇐) is immediate from the definition of convex.

(⇒) Suppose K is a convex subset of \mathbb{R}^n and let x be a convex combination of r points of K. We will show $x \in K$ by induction on r. When r = 2, $x \in K$ by the definition of convex. Let p be a positive integer such that every convex combination of p or fewer points of K lies in K. Let $x = \lambda_1 x_1 + \dots + \lambda_p x_p + \lambda_{p+1} x_{p+1}$ where $\lambda_1 + \dots + \lambda_{p+1} = 1$, $\lambda_i \ge 0$ and $x_i \in K$ for each i. If $\lambda_{p+1} = 1$, then $\lambda_1 = \lambda_2 = \dots = \lambda_p = 0$ since $\lambda_1 + \dots + \lambda_{p+1} = 1$, and $\lambda_i \ge 0$ for each i. Thus $x = x_{p+1} \in K$. If $\lambda_{p+1} < 1$, we have $\lambda_1 + \dots + \lambda_p = 1 - \lambda_{p+1} > 0$.

Hence

$$x = (\lambda_1 + \dots + \lambda_p) \left(\frac{\lambda_1}{\lambda_1 + \dots + \lambda_p} x_1 + \dots + \frac{\lambda_p}{\lambda_1 + \dots + \lambda_p} x_p \right) + \lambda_{p+1} x_{p+1}.$$

By the inductive hypothesis, the point

$$y = \frac{\lambda_1}{\lambda_1 + \dots + \lambda_p} x_1 + \dots + \frac{\lambda_p}{\lambda_1 + \dots + \lambda_p} x_p$$

belongs to K. Thus $x = (1 - \lambda_{p+1})y + \lambda_{p+1}x_{p+1}$ which must lie in K since K is convex.

2.3.3 Definition. The *convex hull* of a set $K \subset \mathbb{R}^n$ is the intersection of all convex sets which contain K. We will write conv(K) to denote the convex hull of K.

Observe that the convex hull of a set is convex.

2.3.4 Lemma. [Lay, 2.22] Let K be a subset of \mathbb{R}^n . Then the convex hull of K consists precisely of all convex combinations of elements of K.

Proof. Let T denote the set of all convex combinations of elements of K. Since conv(K) is convex and $K \subset conv(K)$, Lemma 2.3.2 implies that $T \subset conv(K)$.

Conversely, let $x \equiv \alpha_1 x_1 + \cdots + \alpha_r x_r$ and $y \equiv \beta_1 y_1 + \cdots + \beta_s y_s$ be two elements of T and $\lambda \in (0, 1)$. Then

$$\lambda x + (1 - \lambda)y = \lambda \alpha_1 x_1 + \dots + \lambda \alpha_r x_r + (1 - \lambda)\beta_1 y_1 + \dots + (1 - \lambda)\beta_s y_s$$

is an element of T since each coefficient is between 0 and 1 and

$$\sum_{i=1}^r \lambda \alpha_i + \sum_{j=1}^s (1-\lambda)\beta_j = \lambda \sum_{i=1}^r \alpha_i + (1-\lambda) \sum_{j=1}^s \beta_j = \lambda(1) + (1-\lambda)1 = 1.$$

Thus we have shown that T is a convex set. Since $K \subset T$, it follows that $conv(K) \subset T$. Therefore, conv(K) = T.

- **2.3.5 <u>Definition.</u>** A finite set of points $x_1, ..., x_m$ is affinely dependent if there exist real numbers $\lambda_1, ..., \lambda_m$, not all zero, such that $\lambda_1 + ... + \lambda_m = 0$ and $\lambda_1 x_1 + ... + \lambda_m x_m = 0$.
- **2.3.6** Lemma. [Lay, 2.18] Any subset of \mathbb{R}^n consisting of at least n+2 distinct points is affinely dependent.

Proof. Suppose $x_1, ..., x_m$ are distinct points in \mathbb{R}^n with $m \ge n + 2$. Then the m - 1 vectors $x_2 - x_1, x_3 - x_1, ..., x_m - x_1$ are linearly dependent. Thus there exist scalars $\alpha_2, \alpha_3, ..., \alpha_m$, not all zero, such that $\alpha_2(x_2 - x_1) + \alpha_3(x_3 - x_1) + \cdots + \alpha_m(x_m - x_1) = \theta$.

That is,

$$\begin{aligned} -(\alpha_2+\alpha_3+\cdots+\alpha_m)x_1+\alpha_2x_2+\cdots+\alpha_mx_m&=\theta\\ \text{or}\qquad &\alpha_1x_1+\alpha_2x_2+\cdots+\alpha_mx_m&=\theta,\\ \text{where }\alpha_1=-(\alpha_2+\alpha_3+\cdots+\alpha_m). \text{ Thus }\sum_{i=1}^m\alpha_i&=0, \text{ and the points }x_1,\,x_2,\ldots,\,x_m \text{ are affinely}\\ \text{dependent.} \end{aligned}$$

2.3.7 Theorem. [Lay, 2.23] If K is a nonempty subset of \mathbb{R}^n , then every x in conv(K) can be expressed as a convex combination of n+1 or fewer elements of K. Proof. Let $x \in \text{conv}(K)$. Then Lemma 2.3.4 implies that $x = \lambda_1 x_1 + \dots + \lambda_m x_m$, where m is a positive integer, $\lambda_1 + \lambda_2 + \dots + \lambda_m = 1$, and $\lambda_i \geq 0$ and $x_i \in K$ for each $i = 1, \dots, m$. We will show that such an expression exists for x with $m \leq n+1$.

If m > n + 1, then by Lemma 2.3.6, the points $x_1, ..., x_m$ are affinely dependent, i.e., there exist scalars $\alpha_1, ..., \alpha_m$, not all zero, such that

$$\alpha_1 + \cdots + \alpha_m = 0$$
 and $\alpha_1 x_1 + \cdots + \alpha_m x_m = 0$.

So we have

$$\lambda_1 x_1 + \cdots + \lambda_m x_m = x$$

and

$$\alpha_1 x_1 + \cdots + \alpha_m x_m = \theta$$
.

We will now eliminate one of the x_i by subtracting an appropriate multiple of the second equation from the first, yielding a convex combination of fewer than m elements of K which is equal to x.

Since not all of the α_i are zero, and $\sum_{i=1}^m \alpha_i = 0$, at least one of the α_i must be positive. We may assume without loss of generality that $\alpha_m > 0$. Then $\frac{\lambda_m}{\alpha_m} \ge 0$ since $\lambda_m \ge 0$. Consider the set $\left\{\frac{\lambda_i}{\alpha_i} : \alpha_i > 0\right\}$. Since this set is finite, it must contain a minimal element.

We may assume without loss of generality that $\frac{\lambda_m}{\alpha_m} \le \frac{\lambda_i}{\alpha_i}$ for all those i for which $\alpha_i > 0$.

For
$$i = 1,..., m$$
, let $\beta_i = \lambda_i - \left(\frac{\lambda_m}{\alpha_m}\right)\alpha_i$. Then $\beta_m = 0$ and
$$\sum_{i=1}^m \beta_i = \sum_{i=1}^m \lambda_i - \frac{\lambda_m}{\alpha_m} \sum_{i=1}^m \alpha_i = 1 - 0 = 1.$$

We claim that each $\beta_i \ge 0$. If $\alpha_i \le 0$, then $\beta_i \ge \lambda_i \ge 0$. If $\alpha_i > 0$, then

$$\beta_{i} = \alpha_{i} \left(\frac{\lambda_{i}}{\alpha_{i}} - \frac{\lambda_{m}}{\alpha_{m}} \right) \ge 0. \text{ Thus we have}$$

$$\sum_{i=1}^{m-1} \beta_{i} x_{i} = \sum_{i=1}^{m} \beta_{i} x_{i} = \sum_{i=1}^{m} \left(\lambda_{i} - \frac{\lambda_{m}}{\alpha_{m}} \alpha_{i} \right) x_{i}$$

$$= \sum_{i=1}^{m} \lambda_{i} x_{i} - \frac{\lambda_{m}}{\alpha_{m}} \sum_{i=1}^{m} \alpha_{i} x_{i} = \sum_{i=1}^{m} \lambda_{i} x_{i} = x.$$

Hence we have expressed x as a convex combination of m - 1 of the points $x_1, ..., x_m$. This process may be repeated until we have expressed x as a convex combination of n + 1 of the points $x_1, ..., x_m$.

2.3.8 <u>Lemma</u>. [Lay, 2.30] The convex hull of a compact subset of Rⁿ is compact.

Proof. Let K be a (nonempty) compact subset of ${\bf R}^n$. Define a subset B of ${\bf R}^{n+1}$ by

$$B=\{(\alpha_1,\ldots,\,\alpha_{n+1}):\ \alpha_1+\cdots+\,\alpha_{n+1}=1\ \text{and}\ \alpha_j\geq 0\ \text{for}\ 1\leq j\leq n+1\}.$$

We claim that B is compact. From the definition of B, each entry of any element of B lies between 0 and 1, inclusive. Hence B is bounded. Let $\langle a^{(i)} \rangle = \langle (\alpha_1^{(i)}, ..., \alpha_{n+1}^{(i)}) \rangle$ be a

convergent sequence in B with limit $a^{(0)}$. We will show $a^{(0)} \in B$ which implies any limit point of B lies in B, i.e., B is closed. Since $\langle a^{(i)} \rangle$ converges to $a^{(0)}$, we have $\lim_{i \to \infty} \alpha_j^{(i)} = \alpha_j^{(0)}$

for each
$$j \in \{1,..., n+1\}$$
. Thus

$$\begin{split} \alpha_{1}^{(0)} + \alpha_{2}^{(0)} + \cdots + \alpha_{n+1}^{(0)} &= \lim_{i \to \infty} \alpha_{1}^{(i)} + \lim_{i \to \infty} \alpha_{2}^{(i)} + \cdots + \lim_{i \to \infty} \alpha_{n+1}^{(i)} \\ &= \lim_{i \to \infty} \left[\alpha_{1}^{(i)} + \cdots + \alpha_{n+1}^{(i)} \right] \\ &= \lim_{i \to \infty} \langle 1 \rangle_{i=1}^{\infty} = 1. \end{split}$$

Also since $\alpha_j^{(i)} \ge 0$ for each $i \in \mathbb{N}$ and $j \in \{1,...,n+1\}$, $\alpha_j^{(0)} \ge 0$ for each $j \in \{1,...,n+1\}$. Hence we have shown that $a^{(0)} \in B$ and that B is compact.

The function f defined by

$$\begin{split} &f(\alpha_1,\ldots,\,\alpha_{n+1},\,x_{11},\ldots,\,x_{1n},\,x_{21},\ldots,\,x_{2n},\ldots,\,x_{n+1,1},\ldots,\,x_{n+1,n})\\ &=\sum_{i=1}^{n+1}\alpha_i(x_{i1},\ldots,x_{in}) \end{split}$$

is a continuous mapping of $\mathbb{R}^{n+1} \times \mathbb{R}^n \times \cdots \times \mathbb{R}^n = \mathbb{R}^{(n+1)^2}$ into \mathbb{R}^n .

We claim that $f(B \times K \times \cdots \times K) = conv(K)$. Let $x \in f(B \times K \times \cdots \times K)$. Then by the definition of f, x is a convex combination of elements of K which must be in conv(K) by Lemma 2.3.4. Now let $x \in conv(K)$. Then by Theorem 2.3.7, x can be expressed as a convex combination of n + 1 or fewer elements of K, i.e.,

$$x=\sum_{i=1}^{n+1}\alpha_i(x_{i1},\ldots,x_{in}), \text{ where } \sum_{i=1}^{n+1}\alpha_i=1 \text{ and } \alpha_i\geq 0 \text{ for } 1\leq i\leq n+1.$$

The function f maps $(\alpha_1, \ldots, \alpha_{n+1}, x_{11}, \ldots, x_{1n}, x_{21}, \ldots, x_{2n}, \ldots, x_{n+1,1}, \ldots, x_{n+1,n}) \in$ $B \times K \times \cdots \times K \subset \mathbf{R}^{(n+1)^2} \text{ to } x; \text{ thus } x \in f(B \times K \times \cdots \times K). \text{ Hence we have shown that}$ $f(B \times K \times \cdots \times K) = \text{conv}(K).$

Since B and K are compact, so is the finite direct product $B \times K \times \cdots \times K$ by Tychonoff's Theorem [Pat, 6.50]. It is not hard to prove this compactness here as follows. Since B and K are both bounded, it follows that $B \times K \times \cdots \times K$ is bounded. Let

$$\left\langle y^{(i)} \right\rangle = \left\langle (\alpha_1^{(i)}, \dots, \alpha_{n+1}^{(i)}, x_{11}^{(i)}, \dots, x_{1n}^{(i)}, x_{21}^{(i)}, \dots, x_{2n}^{(i)}, \dots, x_{n+1,1}^{(i)}, \dots x_{n+1,n}^{(i)}) \right\rangle$$

be a convergent sequence in $B \times K \times \cdots \times K$ with limit $y^{(0)}$. We will show $y^{(0)} \in B \times K \times \cdots \times K$. Since $\left\langle y^{(i)} \right\rangle$ converges to $y^{(0)}$, we have $\lim_{i \to \infty} \alpha_j^{(i)} = \alpha_j^{(0)}$ and $\lim_{i \to \infty} x_{jk}^{(i)} = x_{jk}^{(0)}$ for each $j \in \{1, \dots, n+1\}$ and each $k \in \{1, \dots, n\}$. From the argument above showing B is closed, we know $(\alpha_1^{(0)}, \dots, \alpha_{n+1}^{(0)}) \in B$. Also since K is closed, it follows that $(x_{j1}^{(0)}, \dots, x_{jn}^{(0)}) \in K$ for $1 \le j \le n+1$. Thus we have shown that

 $y^{(0)}\!\in\, B\times K\times\!\!\cdots\!\!\times K$ which implies that $B\times K\times\!\!\cdots\!\!\times K$ is closed.

Since the continuous image of a compact set is compact [Pat, 4.19], it now follows that $f(B \times K \times \cdots \times K)$, which is conv(K), is compact.

CHAPTER 3

MAXIMIZING THE DETERMINANT OF THE COMPLETION

3.1 Preliminaries

The following lemma brings together two statements from [GJSW]. The first is needed in the proof of their Theorem 2 (our 3.2.1), and the second is the reason for development of their Theorems 4 and 5 (our 3.3.3 and 3.3.5).

3.1.1 Lemma. Let G be a graph, and let A(G) be a G-partial matrix having a positive semidefinite completion. If G contains all possible loops, then S(A(G)) is bounded and closed, hence compact. If one or more loops is missing in G, then S(A(G)) is closed but not bounded.

Proof. Suppose G contains all possible loops. Then every diagonal entry a_{ii} of A(G) is specified. Let $m = \max\{\sqrt{a_{ii}a_{jj}}: 1 \le i,j \le n\}$. If $Y \in S(A(G))$, then every principal submatrix of Y is positive semidefinite by Theorem 1.1.9; in particular, the 2-by-2 principal submatrices of Y are positive semidefinite. Let $\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix}$ be an arbitrary 2-by-2 principal submatrix of A(G) with a_{ij} (and hence a_{ji}) unspecified. If $\begin{bmatrix} y_{ii} & y_{ij} \\ y_{ji} & y_{ij} \end{bmatrix}$ is the

corresponding submatrix in Y, then we must have $y_{ii}y_{jj} - y_{ij}y_{ji} \ge 0$, i.e., $y_{ii}y_{jj} \ge |y_{ij}|^2$. Thus each entry of Y satisfies $|y_{ij}| \le m$. Since Y was chosen arbitrarily, we have shown that S(A(G)) is bounded. We have already seen that S(A(G)) is closed in H (see 1.2.6); thus we conclude that S(A(G)) is compact.

Suppose the loop $\{k, k\}$ in not an edge in G. Let Y be a positive semidefinite completion of A(G). Obtain Y_t by adding a positive real t to the (k, k)-entry of Y. Then for any nonzero complex vector $\mathbf{x} = [x_1, ..., x_n]^t$, $\mathbf{x}^* Y_t \mathbf{x} = \mathbf{x}^* Y \mathbf{x} + t \overline{\mathbf{x}_k} \mathbf{x}_k \ge \mathbf{x}^* Y \mathbf{x} \ge 0$; so Y_t is positive semidefinite. Since Y_t is a completion of A(G), Y_t is in S(A(G)). And because t can be arbitrarily large, S(A(G)) is not bounded.

Notice that in the course of proving Lemma 3.1.1, we have also proved the following:

3.1.2 Lemma. [HJ, p. 398] Given a positive semidefinite matrix A, each entry a_{ij} of A satisfies $|a_{ij}|^2 \le a_{ii}a_{jj}$. If A is positive definite, the inequality is strict.

3.2 Theorems in which the Graph Contains all Possible Loops

3.2.1 Theorem. [GJSW] Suppose a graph G = (V, E) contains all possible loops and let A(G) be a G-partial matrix having at least one positive definite completion. Then there exists a unique positive definite completion B_0 of A(G) such that

$$det(B_0) = max\{det(Z): Z \in S(A(G))\}.$$

Furthermore, B_0 is the unique positive definite completion of A(G) whose inverse, $C = [c_{kp}]$, satisfies

$$c_{kp} = 0$$
 for all $\{k, p\} \notin E$.

Proof. Let W be a positive definite completion of A(G) and let $0 < \epsilon < \det(W)$. We will apply Theorem 2.2.6, so we need a convex, compact set in S(A(G)) which contains W and on which logdet is defined and strictly concave. Define $K_{\epsilon} = \{Z \in S(A(G)): \det(Z) \ge \epsilon\}$. We will see that conv(K_{ϵ}) has all the necessary properties. The K_{ϵ} notation was not used in [GJSW], but is helpful in substantiating some of the claims there.

We first show that K_{ε} is compact. Since the determinant function is continuous and $[\varepsilon, \infty)$ is closed in \mathbb{R} , it follows that $\{Z \in \mathbb{H}: \det(Z) \geq \varepsilon\}$ is closed in \mathbb{H} . Thus $K_{\varepsilon} = S(A(G)) \cap \{Z \in \mathbb{H}: \det(Z) \geq \varepsilon\}$ is the intersection of closed sets in \mathbb{H} ; hence K_{ε} is closed in \mathbb{H} . Since S(A(G)) is bounded by Lemma 3.1.1, K_{ε} is bounded.

Now since K_{ϵ} is compact, $\operatorname{conv}(K_{\epsilon})$ is compact by Lemma 2.3.8. Also by virtue of its definition, $\operatorname{conv}(K_{\epsilon})$ is convex. In addition, we claim that K_{ϵ} has more than one element since it contains W, and a small enough change in an entry or entries of W corresponding to free entries in A(G) results in another positive definite completion X of A(G) with $\det(X) > \epsilon$. One way to see this is to use the fact that the roots of a polynomial are continuously dependent on the coefficients [HJ, Appendix D] which implies that the eigenvalues of a matrix are continuously dependent on the entries. This assures the existence of another positive definite completion of A(G) in addition to W. Since (ϵ, ∞) is

open in \mathbf{R} and det is continuous, $\det^{-1}(\varepsilon, \infty)$ is open in \mathbf{H} . Thus any positive definite completion of A(G) sufficiently close to W will have determinant greater than ε . Hence we conclude that K_{ε} has more than one element which implies $\operatorname{conv}(K_{\varepsilon})$ has more than one element.

3.2.2 If $U, Y \in S^o(A(G))$ and $t \in (0, 1)$, then tU + (1 - t)Y is positive definite since tU + (1 - t)Y is Hermitian and $x^*(tU + (1 - t)Y)x = tx^*Ux + (1 - t)x^*Yx > 0$ when $x \neq 0$. In addition, tU + (1 - t)Y is a completion of A(G). Hence $tU + (1 - t)Y \in S^o(A(G))$ which proves $S^o(A(G))$ is a convex set. Since $S^o(A(G))$ contains K_{ϵ} , it now follows that $conv(K_{\epsilon}) \subset S^o(A(G))$. Thus det(Z) > 0 for $Z \in conv(K_{\epsilon})$ and by Theorem 2.2.3, the determinant function is strictly log-concave on $conv(K_{\epsilon})$. Therefore the hypotheses of Theorem 2.2.6(i) are satisfied; so there exists a unique $B_0 \in conv(K_{\epsilon})$ such that $det(B_0) = max\{det(Z): Z \in conv(K_{\epsilon})\}$.

If $X \in S(A(G))$ - K_{ϵ} , then $det(X) < \epsilon$; hence the above matrix B_0 is the unique matrix in S(A(G)) with maximum determinant. Since $B_0 \in conv(K_{\epsilon})$, $B_0 \in S^o(A(G))$, the interior of S(A(G)) relative to H(A(G)) [Theorem 1.2.7]. Thus we must have

$$\left(\frac{\partial \det}{\partial x_{kp}}\right)(B_0) = 0 = \left(\frac{\partial \det}{\partial y_{kp}}\right)(B_0)$$
 for all $\{k, p\} \notin E$, where x_{kp} denotes the real part and

 y_{kp} denotes the imaginary part of the (k, p)-entry.

Hence by Theorem 2.2.5, $B_0(k \mid p) = 0$ for $\{k, p\} \notin E$. Letting $B_0^{-1} = C = [c_{kp}]$, we have $C = \frac{1}{\det(B_0)} \operatorname{adj}(B_0)$ (see Part One, 2.1.4 - 2.1.5). Hence

$$c_{kp} = \frac{(-1)^{k+p} B_0(p|k)}{\det(B_0)},$$

and thus $c_{kp} = 0$ for all $\{k, p\} \notin E$. It just remains to show that B_0 is the only positive definite completion of A(G) with this property.

3.2.3 <u>Definition</u>. If we let $Z = [x_{kp} + iy_{kp}]$ represent a general element of S(A(G)), then the (k, p)-entries of Z and A(G) agree for $\{k, p\} \in E$, i.e., x_{kp} and y_{kp} are fixed for $\{k, p\} \in E$. Accordingly, we denote by $(\nabla_G \det)(Z)$ the gradient of the function det: $\mathbf{H}(A(G)) \to \mathbf{R}$, evaluated at Z, where det is a function of the real variables x_{kp} and y_{kp} for $\{k, p\} \notin E$. In particular, $(\nabla_G \det)(B_0)$ will denote $\nabla_G \det$ evaluated at the matrix B_0 .

Observe that the following are equivalent, where $C = [c_{kp}]$ is the inverse of B_0 :

1.
$$c_{kp} = 0$$
 for $\{k, p\} \notin E$

2.
$$0 = B_0(p \mid k) = \overline{B_0(k \mid p)}$$
 for $\{k, p\} \notin E$

3.
$$B_0(k \mid p) = 0$$
 for $\{k, p\} \notin E$

4.
$$\left(\frac{\partial \det}{\partial x_{kp}}\right)(B_0) = \left(\frac{\partial \det}{\partial y_{kp}}\right)(B_0) = 0 \text{ for } \{k, p\} \notin E$$

5.
$$(\nabla_G \det)(B_0) = 0$$

6.
$$(\nabla \det)(\mathbf{B}_0) = 0$$

7.
$$\langle (\nabla \det)(B_0), Z - B_0 \rangle = 0$$
 for every $Z \in S(A(G))$.

To see that item 7 implies 6, recall that B_0 lies in the open set $S^o(A(G))$; thus Z can be chosen in $S^o(A(G))$ so that $Z - B_0$ points in any direction. So we have $\langle (\nabla \det)(B_0), Z - B_0 \rangle = 0$, where $Z - B_0$ can point in any direction, which implies $(\nabla \det)(B_0) = 0$.

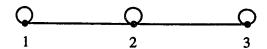
Suppose B' is another positive definite completion of A(G) whose inverse has zeros in the positions corresponding to unspecified entries in A(G). Let $0 < \varepsilon' < \det(B')$ and define $K_{\varepsilon'}$ as before. Then $\det(B_0)$ and $\det(B')$ are both positive and from above,

$$\langle (\nabla \det)(B_0), Z - B_0 \rangle = 0 = \langle (\nabla \det)(B'), Z - B' \rangle$$
 for every $Z \in S(A(G))$.

But by Theorem 2.2.6(ii), B_0 is the unique element of $conv(K_{\epsilon'})$ which satisfies $det(B_0) > 0$ and $\langle (\nabla det)(B_0), Z - B_0 \rangle \leq 0$ for every $Z \in conv(K_{\epsilon'})$. Since B' also satisfies these properties, we have a contradiction. Thus we conclude that B_0 is the only positive

definite completion of A(G) whose inverse has zeros in the positions corresponding to unspecified entries in A(G).

3.2.4 Example. Let G =



and A(G) =
$$\begin{bmatrix} 2 & 1 & x \\ 1 & 2 & 1 \\ \overline{x} & 1 & 1 \end{bmatrix}$$
, where x denotes an unspecified entry.

Then
$$W = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$
 is a positive definite completion, and $B_0 = \begin{bmatrix} 2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 1/2 & 1 & 1 \end{bmatrix}$ is the

unique positive definite completion with maximum determinant on S(A(G)). Furthermore,

$$\mathbf{B}_0^{-1} = \begin{bmatrix} 2/3 & -1/3 & 0 \\ -1/3 & 7/6 & -1 \\ 0 & -1 & 2 \end{bmatrix}, \text{ and it is not hard to check that the inverse of any other}$$

positive definite completion will not have zeros in the (1, 3) and (3, 1) positions.

In the previous theorem, we considered what happens to the determinant function on the set of all positive definite completions of a fixed G-partial matrix A(G). Now in addition, suppose for each unspecified entry in A(G), we require that any number to fill the position must lie on a fixed straight line in the complex plane. Even though this is a strong restriction, the following theorem establishes a similar result to the unrestricted case.

We identify C with \mathbb{R}^2 by $(x + iy) \leftrightarrow (x, y)$.

3.2.5 Theorem. [GJSW] Suppose a graph G = (V, E) contains all possible loops and suppose there exists a G-partial matrix A(G) having a positive definite completion $W = [w_{kp}]$. For each $\{r, s\} \notin E$, fix a straight line L_{rs} in \mathbb{R}^2 such that $w_{rs} \in L_{rs}$. Then there exists a unique B in S(A(G)) such that

$$det(B) = max\{det(Z): Z \in S(A(G)), z_{rs} \in L_{rs} \text{ for each } \{r, s\} \notin E\}.$$

This matrix B is the unique positive definite completion of A(G) whose inverse, $C = [c_{kp}]$, satisfies

$$c_{rs}$$
 is orthogonal to L_{rs} for each $\{r, s\} \notin E$. (*)

(This means orthogonality in \mathbb{R}^2 , i.e., $c_{rs} = a + bi$ corresponds to the point (a, b) in the complex plane, and to say c_{rs} is orthogonal to L_{rs} means $(a, b) \cdot (e, f) = 0$, whenever the line segment joining (e, f) and (0, 0) is parallel to L_{rs} and \bullet denotes the standard inner product on \mathbb{R}^2 .)

Proof. Define $K = \{Z \in S(A(G)): z_{rs} \in L_{rs} \text{ for each } \{r, s\} \notin E\}$. Let $0 < \epsilon < \det(W)$. We will apply Theorem 2.2.6, so we need a convex, compact set in S(A(G)) which contains W and on which logdet is defined and strictly concave. Define

 $K_{\varepsilon} = \{Z \in K: \det(Z) \ge \varepsilon\}$. We will see that $\operatorname{conv}(K_{\varepsilon})$ has all the necessary properties.

Since $W \in K_{\epsilon}$ and a small change in an entry or entries of W results in a small change in its eigenvalues, any $M = [m_{kp}]$ with the properties that $m_{rs} \in L_{rs}$ for each $\{r, s\} \notin E$, $m_{kp} = w_{kp}$ for $\{k, p\} \in E$, and which is sufficiently close to W will also be a positive definite completion of A(G) with determinant greater than ϵ (because $W \in det^{-1}(\epsilon, \infty)$, an open set in H). Hence K_{ϵ} has more than one element.

To show K_{ϵ} is compact, we will show K is closed. Then because K is a subset of S(A(G)), which is compact by Lemma 3.1.1, it follows that K is compact. And since det is continuous, K_{ϵ} is a closed subset of K; hence K_{ϵ} is compact. To see that K is closed in H, let $A^{(1)}$, $A^{(2)}$,... be a convergent sequence of matrices in K with limit $M = [m_{kp}]$. This means $\lim_{i \to \infty} Re(A^{(i)}_{rs}) = Re(m_{rs})$ and $\lim_{i \to \infty} Im(A^{(i)}_{rs}) = Im(m_{rs})$ where $A^{(i)}_{rs}$ denotes the (r, s)-

entry of $A^{(i)}$. In addition, for each $\{r, s\} \notin E$ and $i \in \mathbb{N}$, $A^{(i)}_{rs} \in L_{rs}$. Hence $m_{rs} \in L_{rs}$ since L_{rs} is closed. Furthermore, $M \in S(A(G))$ since S(A(G)) is closed in H. Thus $M \in K$ which proves that K is closed in H.

Now since K_{ε} is compact, $\operatorname{conv}(K_{\varepsilon})$ is compact by Lemma 2.3.8, is convex by virtue of its definition, and has more than one element since K_{ε} does. Since $S^o(A(G))$ is convex (see 3.2.2 in the proof of Theorem 3.2.1) and $K_{\varepsilon} \subset S^o(A(G))$, it follows that $\operatorname{conv}(K_{\varepsilon}) \subset S^o(A(G))$. Thus $\operatorname{conv}(K_{\varepsilon})$ is a compact, convex set satisfying the hypotheses of Theorem 2.2.6(i); so there exists a unique $B \in \operatorname{conv}(K_{\varepsilon})$ such that

 $det(B) = max\{det(Z): Z \in conv(K_{\epsilon})\}.$

If $X \in S(A(G))$ - K_{ϵ} , then $det(X) < \epsilon$; so det(X) < det(B). Hence B is the unique matrix in S(A(G)) such that

 $\det(B) = \max\{\det(Z): \ Z \in S(A(G)), z_{rs} \in L_{rs} \text{ for each } \{r, s\} \notin E\}.$

Since $B \in conv(K_{\varepsilon})$, B must be positive definite.

Now we will prove that B is the only positive definite completion of A(G) whose inverse C has the property (*). By Theorem 2.2.6(ii), B is the unique element of $conv(K_{\epsilon})$ satisfying det(B) > 0 and $\langle (\nabla det)(B), Z - B \rangle \leq 0$ for all $Z \in conv(K_{\epsilon})$. Since ϵ can be chosen arbitrarily close to zero, B is in fact the unique element of $S^o(A(G))$ satisfying $\langle (\nabla det)(B), Z - B \rangle \leq 0$ for all $Z \in K \cap S^o(A(G))$. Let $b_{rs} = \beta_{rs} + i\gamma_{rs}$ denote the (r, s)-entry of B, and let $\frac{\partial det}{\partial x_{rs}}$ and $\frac{\partial det}{\partial y_{rs}}$ denote the partial derivatives of the determinant function with

respect to the real part and imaginary part of the (r, s)-entry, respectively. Then

$$\langle (\nabla \det)(B), Z - B \rangle = \sum_{r,s=1}^{n} \left[\left(\frac{\partial \det}{\partial x_{rs}} \right) (B) \right] \left[\operatorname{Re}(z_{rs}) - \beta_{rs} \right] + \left[\left(\frac{\partial \det}{\partial y_{rs}} \right) (B) \right] \left[\operatorname{Im}(z_{rs}) - \gamma_{rs} \right]$$

$$= \sum_{r,s=1}^{n} 2(-1)^{r+s} [\text{Re}(B(r \mid s))] [\text{Re}(z_{rs}) - \beta_{rs}] + (-2)(-1)^{r+s} [\text{Im}(B(r \mid s))] [\text{Im}(z_{rs}) - \gamma_{rs}]$$
by Theorem 2.2.5

$$= 2 \sum_{\{r,s\} \notin E} (-1)^{r+s} [\text{Re}(B(r \mid s))] [\text{Re}(z_{rs}) - \beta_{rs}] - (-1)^{r+s} [\text{Im}(B(r \mid s))] [\text{Im}(z_{rs}) - \gamma_{rs}]$$
since when $\{r, s\} \in E$, $\text{Re}(z_{rs}) = \beta_{rs}$ and $\text{Im}(z_{rs}) = \gamma_{rs}$.

Thus $\langle (\nabla \det)(B), Z - B \rangle \leq 0$ is equivalent to

$$\sum_{(r,s) \notin E} (-1)^{r+s} [\text{Re}(B(r \mid s))] [\text{Re}(z_{rs}) - \beta_{rs}] - (-1)^{r+s} [\text{Im}(B(r \mid s))] [\text{Im}(z_{rs}) - \gamma_{rs}] \leq 0.$$

If we let $C = [c_{kp}]$ be the inverse of B, then $c_{kp} = \frac{(-1)^{k+p}(B(p \mid k))}{\det(B)}$, and the above can be

written as

$$\det(B) \sum_{\{r,s\} \notin E} [\text{Re}(c_{sr})] [\text{Re}(z_{rs}) - \beta_{rs}] - [\text{Im}(c_{sr})] [\text{Im}(z_{rs}) - \gamma_{rs}] \le 0 \quad \text{or} \quad$$

$$\sum_{\{r,s\}\in E} [\text{Re}(c_{rs})][\text{Re}(z_{rs}) - \beta_{rs}] + [\text{Im}(c_{rs})][\text{Im}(z_{rs}) - \gamma_{rs}] \le 0$$
 for every $Z = [z_{kn}] \in K \cap S^{o}(A(G))$.

Fix $\{r, s\} \notin E$. Consider Z in $K \cap S^0(A(G))$ for which $z_{kp} = b_{kp}$ except in the (r, s) and (s, r) positions. Then (**) becomes

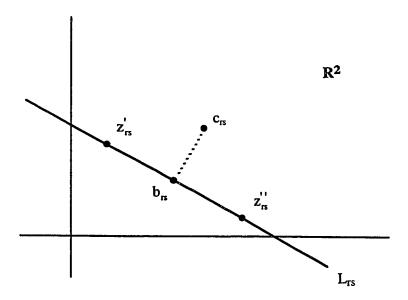
$$\begin{split} [\text{Re}(c_{rs})][\text{Re}(z_{rs}) - \beta_{rs}] + [\text{Im}(c_{rs})][\text{Im}(z_{rs}) - \gamma_{rs}] \\ + [\text{Re}(c_{sr})][\text{Re}(z_{sr}) - \beta_{sr}] + [\text{Im}(c_{sr})][\text{Im}(z_{sr}) - \gamma_{sr}] \leq 0 \end{split}$$

or
$$2\{[Re(c_{rs})][Re(z_{rs}) - \beta_{rs}] + [Im(c_{rs})][Im(z_{rs}) - \gamma_{rs}]\} \le 0.$$

Thus we have

$$\langle c_{rs}, z_{rs} - b_{rs} \rangle \leq 0.$$
 (***)

For each $\{r, s\} \notin E$, (***) holds for all matrices Z in $K \cap S^o(A(G))$ for which $z_{kp} = b_{kp}$ except in the (r, s) and (s, r) positions and where z_{rs} lies on an open segment of L_{rs} containing b_{rs} . Let z'_{rs} , $z''_{rs} \in L_{rs}$ with b_{rs} between them. Then the cosine of the angle between c_{rs} and $z'_{rs} - b_{rs}$ is nonpositive as is the cosine of the angle between c_{rs} and $z'_{rs} - b_{rs}$. Hence each angle must be at least 90° which means each angle must be 90° (see picture).



Since $z'_{rs} - b_{rs}$ and $z''_{rs} - b_{rs}$ have opposite directions along L_{rs} , it follows that c_{rs} is orthogonal to L_{rs} for each $\{r, s\} \notin E$, i.e., $C = B^{-1}$ satisfies property (*).

The fact that B is the unique element of $S^o(A(G))$ whose inverse satisfies property (*) follows because condition (***) occurs if and only if $\langle (\nabla \det)(B), Z - B \rangle \leq 0$ for all $Z \in K \cap S^o(A(G))$. (The work above establishes this.) And since condition (***) is equivalent to property (*), and B is the unique element of $S^o(A(G))$ satisfying $\langle (\nabla \det)(B), Z - B \rangle \leq 0$ for all $Z \in K \cap S^o(A(G))$, it follows that B is the unique element of $S^o(A(G))$ whose inverse satisfies property (*).

3.3 Theorems in which the Graph May be Missing a Loop

3.3.1 So far we have considered only graphs which contain all possible loops. Now suppose we are given a graph G = (V, E) in which the loop $\{k, k\}$ is not in E for some $k \in \{1, ..., n\}$. Suppose $A(G) = [a_{rs}]$ is a G-partial matrix with a positive definite completion $W = [w_{rs}]$, so $S^o(A(G)) \neq \emptyset$. Let $0 < \epsilon < \det(W)$. We showed in Lemma 3.1.1 that S(A(G)) is not bounded, hence not compact. Recall that we defined $K_{\epsilon} = \{Z \in S(A(G)): \det(Z) \geq \epsilon\}$ in Theorem 3.2.1. The compactness of K_{ϵ} was important in establishing the earlier results. However when G is missing a loop (say, $\{k, k\}$), K_{ϵ} is no longer compact. To see this, let W_x be obtained from W by adding x to w_{kk} where x can be any positive real number. Then expanding $\det(W_x)$ about row k, we have

$$\begin{split} \det(W_x) &= w_{k1}(-1)^{k+1}W(k\mid 1) + w_{k2}(-1)^{k+2}W(k\mid 2) + \cdots \\ &+ (w_{kk} + x)(-1)^{k+k}W(k\mid k) + \cdots + w_{kn}(-1)^{k+n}W(k\mid n) \\ &= \det(W) + xW(k\mid k). \end{split}$$

Since x > 0, $xW(k \mid k) > 0$ because $W(k \mid k)$ is a principal minor of the positive definite matrix W; thus $det(W_x) > det(W)$. So $W_x \in K_{\varepsilon}$; and since x can be arbitrarily large, K_{ε} is not bounded and det does not have a maximum on S(A(G)).

However if we restrict attention to a closed and bounded subset K of S(A(G)) which contains a positive definite completion of A(G), then det will have a maximum at some positive definite B in K. Such B cannot be in the interior of K since that would mean $(\nabla \det)(B) = 0$ which implies, since the (k, k)-entry is free, that $\left(\frac{\partial \det}{\partial x_{kk}}\right)(B) = 0$. But by Theorem 2.2.5, $\left(\frac{\partial \det}{\partial x_{kk}}\right)(B)$ is just $B(k \mid k)$, a principal minor of the positive definite B, which must be positive. So when K is any compact subset of S(A(G)), the determinant-maximizing B must occur on the boundary of K. Now fix positive constants T and L and

consider $\{Z \in S(A(G)): tr(Z) \le T\}$ or $\{Z \in S(A(G)): tr(Z^2) \le L\}$. These are compact sets and we will show in each case that the determinant-maximizing B is unique and, as before, that its inverse has an unexpected property.

3.3.2 <u>Lemma.</u> [HJ, p. 398] The diagonal entries of a positive (semi)definite matrix A are all positive (nonnegative).

Proof. Suppose A is positive definite. Let e_k be the $n \times 1$ vector with 1 in the kth position and zeros elsewhere. Then for each $k \in \{1,...,n\}$,

$$0 < e_k^* A e_k$$
 since A is positive definite
= a_{kk} .

Replacing < by \le above gives the proof for positive semidefinite A.

3.3.3 Theorem. [GJSW] Suppose G = (V, E) is a graph in which at least one loop is missing. Fix T > 0 and suppose A(G) is a G-partial matrix with a positive definite completion Z_0 such that $tr(Z_0) \le T$. Let $K = \{Z \in S(A(G)): tr(Z) \le T\}$. Then there exists a unique positive definite B with maximum determinant on K. Furthermore, tr(B) = T and B is the unique element of $\{Z \in S^0(A(G)): tr(Z) = T\}$ whose inverse, $C = [c_{kp}]$, satisfies

$$c_{kp} = 0$$
 for all $\{k, p\} \notin E, k \neq p$,

$$c_{kk} = c_{pp}$$
 for all $\{k, k\}, \{p, p\} \notin E$.

Proof. Let $0 < \epsilon < \det(Z_0)$. We will apply Theorem 2.2.6, so we need a convex, compact set in S(A(G)) which contains Z_0 and on which logdet is defined and strictly concave. Define $K_{\epsilon} = \{Z \in S(A(G)): \det(Z) \geq \epsilon \text{ and } \operatorname{tr}(Z) \leq T\}$. We will see that $\operatorname{conv}(K_{\epsilon})$ has all the necessary properties.

We claim that K_{ϵ} has more than one element. Recalling that the eigenvalues of a matrix are continuously dependent on the entries and det is a continuous function, it follows that

we can make small changes in entries of Z_0 corresponding to unspecified positions in A(G) to obtain another Hermitian completion X of A(G) with positive eigenvalues and $\det(X) > \varepsilon$. Since the eigenvalues of X are positive, X is positive definite. Since there is an unspecified diagonal entry in A(G), and the corresponding entry in Z_0 is positive by Lemma 3.3.2, we may obtain X from Z_0 by decreasing this entry slightly. Then $\operatorname{tr}(X) < \operatorname{tr}(Z_0) \le T$ so that $X \in K_\varepsilon$. Thus we have shown that K_ε has more than one element.

We claim that K_{ϵ} is compact. Since Trace: $\mathbf{H} \to \mathbf{R}$ is continuous and $(-\infty, T]$ is closed in \mathbf{R} , $\{Z \in \mathbf{H}: \operatorname{tr}(Z) \leq T\}$ is closed in \mathbf{H} . Since $K = S(A(G)) \cap \{Z \in \mathbf{H}: \operatorname{tr}(Z) \leq T\}$, the intersection of closed sets in \mathbf{H} , K must be closed in \mathbf{H} . Now $K_{\epsilon} = K \cap \{Z \in \mathbf{H}: \det(Z) \geq \epsilon\}$ is the intersection of closed sets in \mathbf{H} ; hence K_{ϵ} is closed in \mathbf{H} . If $Z = [z_{kp}] \in K$, Z is positive semidefinite so its diagonal entries are nonnegative by Lemma 3.3.2. Thus $z_{kk} \leq \operatorname{tr}(Z) \leq T$. Furthermore, each entry z_{ij} of Z satisfies $|z_{ij}|^2 \leq z_{ii}z_{jj}$ by Lemma 3.1.2. Hence $|z_{ij}| \leq T$, i.e., each entry of Z is bounded. Thus K must be bounded which implies its subset K_{ϵ} is bounded. Therefore we have shown that K_{ϵ} is compact.

So $\operatorname{conv}(K_{\epsilon})$ is compact by Lemma 2.3.8, is convex by virtue of its definition, and has more than one element since K_{ϵ} does. Since $S^o(A(G))$ is convex (see 3.2.2 in the proof of Theorem 3.2.1) and $K_{\epsilon} \subset S^o(A(G))$, it follows that $\operatorname{conv}(K_{\epsilon}) \subset S^o(A(G))$. Thus $\operatorname{conv}(K_{\epsilon})$ is a compact, convex set satisfying the hypotheses of Theorem 2.2.6(i); so there exists a unique $B \in \operatorname{conv}(K_{\epsilon})$ such that

 $det(B) = max\{det(Z): Z \in conv(K_{\epsilon})\}.$

We claim that $tr(B) \le T$. This follows if we can show that the set

 $F = \{Z \in S^o(A(G)): tr(Z) \le T\}$ is convex. Then because F contains K_{ϵ} , F must contain $conv(K_{\epsilon})$, hence $tr(B) \le T$. To see that F is convex, let U, $Y \in F$ and $t \in (0, 1)$. Then $tr(tU + (1 - t)Y) = t \cdot tr(U) + (1 - t)tr(Y) \le tT + (1 - t)T = T$. Since $S^o(A(G))$ is convex,

 $tU + (1 - t)Y \in F$ which implies F is convex.

If $X \in S(A(G))$ - K_{ϵ} , then $det(X) < \epsilon$; so det(X) < det(B). Hence B is the unique matrix in $S^{o}(A(G))$ with maximum determinant among those satisfying $tr(Z) \le T$.

To show that tr(B) = T, suppose tr(B) < T. Then we could increase any diagonal entry of B corresponding to an unspecified position in A(G) until the trace of the resulting matrix B_1 equals T. By the discussion 3.3.1 preceding this theorem, $det(B_1) > det(B)$; but $B_1 \in S^o(A(G))$, and B has maximum determinant on $\{Z \in S^o(A(G)): tr(Z) \le T\}$. Hence we conclude that the trace of B must be T.

So B is on the boundary of K relative to $\mathbf{H}(A(G))$ (where the equation describing the boundary is $b(Z) \equiv tr(Z) - T = 0$). We wish to apply the Lagrange Multiplier Theorem [BL, 4.9.7]. Observe that b and the determinant function are differentiable at B. In addition, because $b(Z) = (\sum_{i=1}^{n} x_{ii}) - T$, $\left(\frac{\partial b}{\partial x_{kk}}\right)(B) = 1$ for each $\{k, k\} \notin E$. Thus

 $(\nabla b)(B) \neq 0$. So because B is an extremal point of the determinant function on K, and hence on the boundary of K, B satisfies

$$(\nabla \det)(B) = \lambda(\nabla b)(B)$$
 for some $\lambda \in \mathbb{R}$ [BL, 4.9.7].

Since B is the unique extremal point of the determinant function on

 $\{Z \in S^o(A(G)): tr(Z) \le T\}$, B is the unique element of $S^o(A(G))$ among those satisfying $tr(Z) \le T$ such that $(\nabla \det)(B) = \lambda(\nabla b)(B)$. In particular, this equality is true for all the real variables corresponding to unspecified positions in A(G), i.e., using our earlier notation, $(\nabla_G \det)(B) = \lambda(\nabla_G b)(B)$.

Thus for each $\{k, k\} \notin E$, we have

$$B(k \mid k) = \left(\frac{\partial \det}{\partial x_{kk}}\right) (B) \quad \text{by Theorem 2.2.5}$$

$$= \lambda \left(\frac{\partial b}{\partial x_{kk}}\right) (B)$$

$$= \lambda \quad \text{since } b(Z) = (\sum_{i=1}^{n} x_{ii}) - T.$$

Furthermore for each $\{k, p\} \notin E, k \neq p$, we have

(i)
$$2(-1)^{k+p} \operatorname{Re}(B(k \mid p)) = \left(\frac{\partial \det}{\partial x_{kp}}\right) (B)$$
 by Theorem 2.2.5
$$= \lambda \left(\frac{\partial b}{\partial x_{kp}}\right) (B)$$

$$= 0, \text{ and}$$

(ii)
$$-2(-1)^{k+p} \operatorname{Im}(B(k \mid p)) = \left(\frac{\partial \det}{\partial y_{kp}}\right) (B)$$
 by Theorem 2.2.5
$$= \lambda \left(\frac{\partial b}{\partial y_{kp}}\right) (B)$$

$$= 0$$

Hence $B(k \mid p) = 0$ for each $\{k, p\} \notin E$, $k \neq p$.

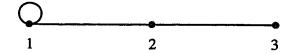
The (k, p)-entry of $B^{-1} = C = [c_{kp}]$ is $\frac{(-1)^{k+p}B(p \mid k)}{\det(B)}$; therefore we must have

(§)
$$c_{kp} = 0 \text{ for each } \{k, p\} \notin E, k \neq p, \text{ and}$$
$$c_{kk} = \frac{\lambda}{\det(B)} \text{ for each } \{k, k\} \notin E.$$

In particular, if $k \neq p$, and $\{k, k\}$, $\{p, p\} \notin E$, then $c_{kk} = c_{pp}$.

Recalling that B is the unique element of $\{Z \in S^o(A(G)): tr(Z) \le T\}$ satisfying $(\nabla_G \det)(B) = \lambda(\nabla_G b)(B)$, and tr(B) = T, it follows that B is the unique element of $\{Z \in S^o(A(G)): tr(Z) = T\}$ whose inverse satisfies (§).

3.3.4 Example. Let G =



and A(G) = $\begin{bmatrix} 1 & 1 & x \\ 1 & y & 1 \\ \overline{x} & 1 & z \end{bmatrix}$, where x, y and z denote unspecified entries, and let T = 5.

Then $Z_0 = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}$ is a positive definite completion such that $tr(Z_0) \le T$, and

 $B = \begin{bmatrix} 1 & 1 & -1 + \sqrt{2} \\ 1 & 1 + \sqrt{2} & 1 \\ -1 + \sqrt{2} & 1 & 3 - \sqrt{2} \end{bmatrix}$ is the unique positive definite completion with

maximum determinant on $\{Z \in S(A(G)): tr(Z) \le T\}$. Furthermore, tr(B) = T and

 $B^{-1} = \begin{vmatrix} 1 + \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{2} + \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} \\ 0 & -\frac{1}{2} & \frac{1}{2} + \frac{1}{2\sqrt{2}} \end{vmatrix}$, and it is not hard to check that B is the unique

element of $\{Z \in S^0(A(G)): tr(Z) = T\}$ whose inverse satisfies conditions (§). We note that other positive definite completions exist with trace less than T and whose inverses satisfy conditions (§). For instance, consider the positive definite completion $\begin{bmatrix} 1 & 2 & 1 \\ 0.5 & 1 & 1.25 \end{bmatrix}$.

In the final result of this chapter, we characterize the determinant-maximizing matrix over another compact subset of positive semidefinite completions with a trace constraint.

- **3.3.5** Theorem. [GJSW] Fix L > 0. Suppose G = (V, E) is a graph, and A(G) is a G-partial matrix with a positive definite completion $W = [w_{kp}]$ subject to $tr(W^2) \le L$. Let $K = \{Z \in S(A(G)): tr(Z^2) \le L\}$. Then there are three possibilities.
- (1) If G has all possible loops and the matrix B_0 from Theorem 3.2.1 is in K, that is, $tr(B_0^2) \le L$, then $det(B_0) = max\{det(Z): Z \in K\}$.
- (2) If G has all possible loops, B_0 from Theorem 3.2.1 is not in K, $w_{kp} = 0$ for all $\{k, p\} \notin E$, and $tr(W^2) = L$, then $K = \{W\}$. In this case, the entries of W⁻¹ corresponding to unspecified positions in A(G) need not be zero.
- (3) If cases (1) and (2) do not hold, then the maximum determinant on K occurs at a positive definite $B = [b_{kp}]$ uniquely determined by

$$tr(B^2) = L$$
 and
 $c_{kp} = \frac{2\lambda b_{kp}}{\det(B)}$ for all $\{k, p\} \notin E$,

where λ is a positive constant and $C = [c_{kp}]$ is the inverse of B.

Proof of (1). Suppose G has all possible loops and the matrix B_0 from Theorem 3.2.1 is in K. Recall that the matrix B_0 from Theorem 3.2.1 has the maximum determinant over all positive semidefinite completions of A(G). Since $B_0 \in K$ and $K \subset S(A(G))$, it follows that B_0 has the maximum determinant on K.

Proof of (2). Suppose case (1) does not hold, G has all possible loops, $w_{kp} = 0$ for all $\{k, p\} \notin E$, and $tr(W^2) = L$. Let $X \in S(A(G))$ and $X \neq W$. We will show $X \notin K$. Because X is Hermitian, $tr(X^2) = tr(X^*X)$ which is the sum of the squares of the moduli of the entries of X. Hence since $w_{kp} = 0$ for all $\{k, p\} \notin E$, $tr(X^2) > tr(W^2) = L$.

Thus $K = \{W\}$. To see that the entries of W-1 corresponding to unspecified positions in A(G) need not be zero, consider the following example.

$$G = \bigcirc \bigcirc \bigcirc \bigcirc$$

$$1 \qquad 2 \qquad 3$$

$$A(G) = \begin{bmatrix} 2 & 1 & x \\ 1 & 2 & 1 \\ \overline{x} & 1 & 1 \end{bmatrix}, \text{ where x denotes an unspecified position; } W = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix}; \text{ and } L = 13. \text{ Then W is positive definite and } W^{-1} = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 2 & -2 \\ 1 & -2 & 3 \end{bmatrix}.$$

L = 13. Then W is positive definite and W-1 =
$$\begin{bmatrix} 1 & -1 & 1 \\ -1 & 2 & -2 \\ 1 & -2 & 3 \end{bmatrix}$$

Proof of (3). Suppose cases (1) and (2) do not hold. Recalling that we are given a positive definite completion $W = [w_{kp}]$ of A(G) subject to $tr(W^2) \le L$, let $0 < \epsilon < det(W)$. We will apply Theorem 2.2.6, so we need a convex, compact set in S(A(G)) which contains W and on which logdet is defined and strictly concave. Define

$$K_{\epsilon} = \{Z \in S(A(G)): \det(Z) \ge \epsilon \text{ and } \operatorname{tr}(Z^2) \le L\}.$$

We will see that $conv(K_{\varepsilon})$ has all the necessary properties.

We first show that K_{ε} contains more than one element. Recalling that the eigenvalues of a matrix are continuously dependent on the entries and det is a continuous function, it follows that small enough changes in entries of W corresponding to unspecified positions in A(G) will yield another Hermitian completion X of A(G) with positive eigenvalues and $det(X) > \varepsilon$. Since the eigenvalues of X are positive, X is positive definite. We claim that such an X exists which satisfies $tr(X^2) \le L$. Since we are assuming case (2) does not hold, there are three possibilities.

- (i) Suppose that $\{k, k\} \notin E$ for some $k \in \{1, ..., n\}$. Then we obtain X from W by decreasing the (k, k)-entry of W.
 - (ii) Suppose G has all possible loops and $w_{kp} \neq 0$ (hence $w_{pk} \neq 0$) for some $\{k, p\} \notin E$.

Then we obtain X from W by changing w_{kp} and w_{pk} so that their modulus is decreased.

(iii) Suppose G has all possible loops, $w_{kp} = 0$ for all $\{k, p\} \notin E$, but $tr(W^2) < L$. Then we may obtain X from W by making small enough changes to w_{kp} (and w_{pk}) for any $\{k, p\} \notin E$ so that $tr(X^2) \le L$.

In each of (i)-(iii) above, we obtained an X satisfying $tr(X^2) \le L$. Thus $X \in K_{\epsilon}$ which implies that K_{ϵ} has more than one element.

Next we show K_{ϵ} is compact. The function $\operatorname{tr}(Z^2)$: $\mathbf{H} \to \mathbf{R}$ is continuous since the trace of the square of a Hermitian matrix is just the sum of the squares of the moduli of its entries. Thus $\{Z \in \mathbf{H} \colon \operatorname{tr}(Z^2) \leq L\}$ is closed in \mathbf{H} since $(-\infty, L]$ is closed in \mathbf{R} . Hence $K = S(A(G)) \cap \{Z \in \mathbf{H} \colon \operatorname{tr}(Z^2) \leq L\}$ is the intersection of closed sets in \mathbf{H} which implies K is closed in \mathbf{H} . So $K_{\epsilon} = K \cap \{Z \in \mathbf{H} \colon \operatorname{det}(Z) \geq \epsilon\}$ is also the intersection of closed sets in \mathbf{H} ; thus K_{ϵ} is closed in \mathbf{H} . Since $\operatorname{tr}(Z^2)$ is the sum of the squares of the moduli of the entries of \mathbf{Z} , each entry \mathbf{z}_{ij} of \mathbf{Z} satisfies $|\mathbf{z}_{ij}|^2 \leq \operatorname{tr}(Z^2) \leq L$. Thus K is bounded and so is its subset K_{ϵ} . Hence we have shown K_{ϵ} is compact.

Therefore $\operatorname{conv}(K_{\epsilon})$ is compact by Lemma 2.3.8, is convex by virtue of its definition, and has more than one element since K_{ϵ} does. Since $S^{o}(A(G))$ is convex (see 3.2.2 in the proof of Theorem 3.2.1) and $K_{\epsilon} \subset S^{o}(A(G))$, it follows that $\operatorname{conv}(K_{\epsilon}) \subset S^{o}(A(G))$. Thus $\operatorname{conv}(K_{\epsilon})$ is a compact, convex set satisfying the hypotheses of Theorem 2.2.6(i); so there exists a unique $B \in \operatorname{conv}(K_{\epsilon})$ such that

To see that $\operatorname{tr}(B^2) \leq L$, we will show K is convex; then since $K_{\epsilon} \subset K$, it will follow that $\operatorname{conv}(K_{\epsilon}) \subset K$ which implies $\operatorname{tr}(B^2) \leq L$. To show K is convex, we will use the Frobenius norm on the $n \times n$ matrices. This is defined for an $n \times n$ matrix $A = [a_{kp}]$ as $\|A\|_F = \left(\sum_{k,p=1}^n \left|a_{kp}\right|^2\right)^{1/2}$ where the nonnegative square root is taken on the right-hand side.

 $det(B) = max\{det(Z): Z \in conv(K_{\epsilon})\}.$

The Frobenius norm satisfies all matrix norm properties [HJ, pp. 290-1]. Also since $tr(A^*A) = \sum_{k,p=1}^{n} |a_{kp}|^2$, we have

 $\|A\|_F = [\operatorname{tr}(A^*A)]^{1/2}$ which equals $[\operatorname{tr}(A^2)]^{1/2}$ when A is Hermitian. Let U, Y \in K, t \in (0, 1), and $\theta \neq x \in \mathbb{C}^n$. Then $x^*(tU + (1 - t)Y)x = tx^*Ux + (1 - t)x^*Yx \ge 0$ since U and Y are positive semidefinite. Hence $tU + (1 - t)Y \in S(A(G))$. Also we have

$$\begin{split} (\operatorname{tr}\{[tU+(1-t)Y]^2\})^{1/2} &= \|tU+(1-t)Y\|_F \\ &\leq \|tU\|_F + \|(1-t)Y\|_F \quad \text{matrix norm property} \\ &= t\|U\|_F + (1-t)\|Y\|_F \quad \text{matrix norm property} \\ &= t[\operatorname{tr}(U^2)]^{1/2} + (1-t)[\operatorname{tr}(Y^2)]^{1/2} \\ &\leq tL^{1/2} + (1-t)L^{1/2} \quad \text{since } \operatorname{tr}(U^2), \operatorname{tr}(Y^2) \leq L \\ &= L^{1/2}. \end{split}$$

Hence $tr\{[tU + (1 - t)Y]^2\} \le L$. So $tU + (1 - t)Y \in K$ which implies K is convex.

Thus we have shown that B is the unique matrix with maximum determinant in $\operatorname{conv}(K_{\epsilon})$ and $\operatorname{tr}(B^2) \leq L$. If $X \in S(A(G)) - K_{\epsilon}$, then $\det(X) < \epsilon$; so $\det(X) < \det(B)$. Hence B is the unique matrix in $S^o(A(G))$ with maximum determinant among those satisfying $\operatorname{tr}(Z^2) \leq L$.

To see that $tr(B^2) = L$, suppose $tr(B^2) < L$. If G does not contain all possible loops, then we could increase a diagonal entry of B corresponding to an unspecified position in A(G) obtaining a positive definite completion B_1 with $tr(B_1^2) = L$. Then by the discussion 3.3.1, $det(B_1) > det(B)$, a contradiction. If G contains all possible loops, then B_0 from Theorem 3.2.1 exists, and $tr(B_0^2) > L$ since we are proving case (3) of this theorem (hence assuming case (1) does not hold). Recalling that $K = \{Z \in S(A(G)): tr(Z^2) \le L\}$, the boundary of K relative to S(A(G)), bd(K), is $\{Z \in S(A(G)): tr(Z^2) = L\}$. Since K is closed, $K = int(K) \cup bd(K)$ where int(K) denotes the interior of K relative to S(A(G)).

Since we are assuming $tr(B^2) < L$, $B \in int(K)$. But the proof of Theorem 2.2.6 implies that the determinant function is strictly increasing as you move from B to B_0 along the segment $\{tB_0 + (1 - t)B: 0 \le t \le 1\}$. So there would be B_1 on this segment and in K with $det(B_1) > det(B)$, a contradiction. Thus $tr(B^2) = L$. Hence $B \in bd(K)$ (where the equation describing the boundary is $b(Z) \equiv tr(Z^2) - L = 0$).

We wish to apply the Lagrange Multiplier Theorem [BL, 4.9.7]. Observe that the determinant function and $b(Z) = tr(Z^2) - L$ are differentiable. Because $tr(B^2) = L$ and we are proving case (3) of this theorem (hence assuming case (2) does not hold), we must have condition (i) or (ii) from above (see bottom of p. 80). That is, there exists $\{k, k\} \notin E$, or there exists $\{k, p\} \notin E$ with $b_{kp} \neq 0$. This allows us to conclude that $(\nabla b)(B) \neq 0$, where $b(Z) = tr(Z^2) - L$, by the following calculations.

For each $\{k, k\} \notin E$ (if any),

$$\left(\frac{\partial b}{\partial x_{kk}}\right)(B) = \left[\frac{\partial}{\partial x_{kk}} [tr(Z^2) - L]\right](B)$$

$$= \left[\frac{\partial}{\partial x_{kk}} \sum_{r,s=1}^{n} |z_{rs}|^2\right](B)$$

$$= \left[\frac{\partial}{\partial x_{kk}} |z_{kk}|^2\right](B)$$

$$= \left[\frac{\partial}{\partial x_{kk}} |x_{kk}|^2\right](B)$$

$$= 2b_{kk}.$$

Also for each $\{k, p\} \notin E, k \neq p$,

$$\left(\frac{\partial b}{\partial x_{kp}}\right)(B) = \left[\frac{\partial}{\partial x_{kp}} \left[tr(Z^2) - L\right]\right](B)$$

$$= \left[\frac{\partial}{\partial x_{kp}} \sum_{r,s=1}^{n} \left|z_{rs}\right|^2\right](B)$$

$$= \left[\frac{\partial}{\partial x_{kp}} \left(\left|z_{kp}\right|^2 + \left|z_{pk}\right|^2\right)\right](B)$$

$$= \left[\frac{\partial}{\partial x_{kp}} \left(x_{kp}^2 + y_{kp}^2 + x_{pk}^2 + y_{pk}^2\right)\right](B)$$

$$= \left[\frac{\partial}{\partial x_{kp}} 2x_{kp}^2\right](B)$$

$$= 4Re(b_{kp}).$$

Similarly, for each $\{k, p\} \notin E, k \neq p$,

$$\left(\frac{\partial b}{\partial y_{kp}}\right)(B) = \left[\frac{\partial}{\partial y_{kp}}[tr(Z^2) - L]\right](B)$$
$$= \left[\frac{\partial}{\partial y_{kp}}(2x_{kp}^2 + 2y_{kp}^2)\right](B)$$
$$= 4Im(b_{kp}).$$

If there exists $\{k, k\} \notin E$, then since B is positive definite, $b_{kk} > 0$ by Lemma 3.3.2. Thus $\left(\frac{\partial b}{\partial x_{kk}}\right)(B) > 0$ from above. If there exists $\{k, p\} \notin E$ with $b_{kp} \neq 0$, then $Re(b_{kp}) \neq 0$ or

 $\operatorname{Im}(b_{kp}) \neq 0$ (or both). So at least one of $\left(\frac{\partial b}{\partial x_{kp}}\right)$ (B) or $\left(\frac{\partial b}{\partial y_{kp}}\right)$ (B) is nonzero from above.

Thus $(\nabla b)(B) \neq 0$.

Therefore, because B is an extremal point of the determinant function on K, and hence on the boundary of K, B satisfies

 $(\nabla \det)(B) = \lambda(\nabla b)(B)$ for some $\lambda \in \mathbb{R}$ [BL, 4.9.7].

Since B is the unique extremal point of the determinant function on

 $\{Z \in S^o(A(G)): \operatorname{tr}(Z^2) \le L\}$, B is the unique element of $S^o(A(G))$ among those satisfying $\operatorname{tr}(Z^2) \le L$ such that $(\nabla \det)(B) = \lambda(\nabla b)(B)$. In particular, this equality is true for all the real variables corresponding to unspecified positions in A(G), i.e., using our earlier notation, $(\nabla_G \det)(B) = \lambda(\nabla_G b)(B)$.

Thus for each $\{k, k\} \notin E$ (if any),

$$B(k \mid k) = \left(\frac{\partial \det}{\partial x_{kk}}\right) (B) \quad \text{by Theorem 2.2.5}$$

$$= \lambda \left(\frac{\partial b}{\partial x_{kk}}\right) (B)$$

$$= \lambda \cdot 2b_{kk} \quad \text{from above.}$$

Note that since B is positive definite, λ must be positive.

In addition, for each $\{k, p\} \notin E, k \neq p$,

$$2(-1)^{k+p} \operatorname{Re}(B(k \mid p)) = \left(\frac{\partial \det}{\partial x_{kp}}\right) (B) \quad \text{by Theorem 2.2.5}$$
$$= \lambda \left(\frac{\partial b}{\partial x_{kp}}\right) (B)$$

= $\lambda \cdot 4 \text{Re}(b_{kp})$ from above.

Similarly, for each $\{k, p\} \notin E, k \neq p$,

$$-2(-1)^{k+p} \operatorname{Im}(B(k \mid p)) = \left(\frac{\partial \det}{\partial y_{kp}}\right) (B) \qquad \text{by Theorem 2.2.5}$$

$$= \lambda \left(\frac{\partial b}{\partial y_{kp}}\right) (B)$$

$$= \lambda \cdot 4 \operatorname{Im}(b_{kp}) \qquad \text{from above.}$$

If
$$B^{-1} = C = [c_{rs}]$$
, then for each $\{k, p\} \notin E$,

$$\begin{split} c_{kp} &= \frac{1}{\det(B)} (-1)^{k+p} [\text{Re}(B(p \mid k)) + i \text{Im}(B(p \mid k))] \quad \text{since } B^{-1} = \frac{1}{\det(B)} \text{adj}(B) \\ & \qquad \qquad \qquad \qquad \text{(see Part One, 2.1.4 - 2.1.5)} \\ &= \frac{1}{\det(B)} (-1)^{k+p} [\text{Re}(B(k \mid p)) - i \text{Im}(B(k \mid p))] \quad \text{since } B(p \mid k) = \overline{B(k \mid p)} \\ &= \frac{1}{\det(B)} \cdot 2\lambda \Big[\text{Re}(b_{kp}) + i \text{Im}(b_{kp}) \Big] \qquad \qquad \text{from above} \\ &= \frac{2\lambda}{\det(B)} \cdot b_{kp}. \end{split}$$

Notice that this holds even when k=p: $c_{kk}=\frac{1}{\det(B)}(-1)^{k+k}B(k\mid k)$ which equals $\frac{1}{\det(B)}\cdot 2\lambda b_{kk} \text{ from above.}$

Finally, since B is the unique positive definite element of K satisfying $(\nabla_G \det)(B) = \lambda(\nabla_G b)(B), \text{ and } \operatorname{tr}(B^2) = L, \text{ it follows that B is the unique positive definite element of K satisfying } \operatorname{tr}(B^2) = L \text{ and } c_{kp} = \frac{2\lambda}{\det(B)} \cdot b_{kp} \text{ for all } \{k, p\} \not\in E, \text{ where } \lambda \text{ is a positive constant and } C = [c_{kp}] \text{ is the inverse of B}.$

CHAPTER 4

CHARACTERIZATION OF COMPLETABILITY

4.1 Completable Graphs

- **4.1.1** Given a graph G = (V, E), recall that a clique is a subset C of V for which $\{x, y\} \in E$ for all $x, y \in C$, including all loops $\{x, x\}$ for $x \in C$. The graph G is called *complete* if V is a clique. A *subgraph* of G is a graph (V', E') where $E' \subseteq E$ and $V' \subseteq V$. Also recall that a G-partial positive (semi)definite matrix is a G-partial Hermitian matrix in which every completely specified principal submatrix is positive (semi)definite.
- **4.1.2** <u>Definition</u>. A graph G is *completable* if every G-partial positive definite matrix has a positive definite completion.
- **4.1.3** Definition. Given a graph G = (V, E) and $A \subseteq V$, the graph on A induced by G is the subgraph G(A) = (A, E(A)), where $E(A) = \{\{x, y\} \in E: x, y \in A\}$.

4.1.4 Lemma. [HJ, p. 399] Let A be an $n \times n$ complex matrix. Then A is positive definite if and only if C^*AC is positive definite for some invertible C.

Proof. If A is positive definite, let C = I. If $C^*AC = B$ is positive definite for some invertible C, then $A = (C^*)^{-1}BC^{-1} = (C^{-1})^*BC^{-1}$. Hence A is Hermitian because B is. If x is a nonzero vector in \mathbb{C}^n , $C^{-1}x \neq 0$ because C^{-1} is nonsingular, and we have

$$x^*Ax = (C^{-1}x)^*B(C^{-1}x) > 0.$$

The following result justifies a claim from [GJSW].

4.1.5 Theorem. Let
$$M(x) = \begin{bmatrix} A & B \\ B^* & H + xI \end{bmatrix}$$
, where A is positive definite, H is

Hermitian, and B is any complex matrix of appropriate size. Then there exists a positive y such that M(y) is positive definite.

Proof. Let
$$C = \begin{bmatrix} I & -A^{-1}B \\ 0 & I \end{bmatrix}$$
. Then $C^* = \begin{bmatrix} I & 0 \\ -B^*A^{-1} & I \end{bmatrix}$ and $C^*M(x)C = \begin{bmatrix} A & 0 \\ 0 & H + xI - B^*A^{-1}B \end{bmatrix}$. Since H and $B^*A^{-1}B$ are Hermitian, $H - B^*A^{-1}B$ is

Hermitian. Let y be a positive number greater than the absolute value of the minimal eigenvalue of $H - B^*A^{-1}B$. Then $(H - B^*A^{-1}B) + yI$ has all positive eigenvalues, hence is positive definite.

Since the eigenvalues of a block diagonal matrix are the eigenvalues of its diagonal blocks taken together, and A is positive definite by hypothesis, $C^*M(y)C$ is positive definite. Hence M(y) is positive definite by Lemma 4.1.4.

4.1.6 Proposition. [GJSW] Let L be the set of vertices of a graph G = (V, E) which have loops. Then G is completable if and only if the graph on L induced by G is completable.

Proof. Suppose G is completable. If $L = \emptyset$, the conclusion is true vacuously. Otherwise, let G' denote the graph on L induced by G. We may suppose $L = \{1, ..., k\}$ for some $k \in \{1, ..., n\}$. (If the vertices start out ordered differently, a suitable permutation similarity of any G-partial Hermitian matrix A(G) is equivalent to reordering the vertices of G so that $L = \{1, ..., k\}$. This yields a new G-partial Hermitian matrix A(G) whose leading $k \times k$ principal submatrix is G'-partial Hermitian. And since similar matrices have the same eigenvalues, A(G) will have a positive definite completion if and only if A(G) has a positive definite completion.)

Let A' be a G'-partial positive definite matrix. We want to show that A' has a positive definite completion. Let $A = [a_{ij}]$ be the G-partial matrix with A' as its leading $k \times k$ principal submatrix and $a_{ij} = 0$ for every $\{i, j\} \in E$ such that $\max\{i, j\} > k$. Since any clique must be contained in L, all completely specified principal submatrices of A must be principal submatrices of A', hence must be positive definite because A' is G'-partial positive definite. Thus A is G-partial positive definite. Since G is completable, A has a positive definite completion whose leading $k \times k$ principal submatrix is a positive definite completion of A'. Since A' was chosen arbitrarily, we conclude that G' is completable.

For the converse, suppose G', the graph on L induced by G, is completable. Let A(G) be a G-partial positive definite matrix. If $L = \emptyset$, let H be any Hermitian completion of A(G). Then H + xI is positive definite whenever x is greater than the absolute value of the minimal eigenvalue of H. Hence for such x, H + xI is a positive definite completion of A(G) which implies that G is completable.

If $L \neq \emptyset$, we may assume without loss of generality that $L = \{1, ..., k\}$ for some

 $k \in \{1,...,n\}$ by the permutation similarity argument above. Then the leading $k \times k$ principal submatrix of A(G) must be G'-partial positive definite. Let A' be a positive definite completion of this leading principal submatrix. Let A be any Hermitian completion of A(G) with A' as its leading $k \times k$ principal submatrix. So $A = \begin{bmatrix} A' & B \\ B^* & H \end{bmatrix}$ where H is Hermitian. By Theorem 4.1.5, there exists a positive x such that $A(x) = \begin{bmatrix} A' & B \\ B^* & H + xI \end{bmatrix}$ is positive definite. Since A(x) is a completion of A(G), we conclude that G is completable.

In view of Proposition 4.1.6, we will henceforth assume L = V, i.e., that every vertex in a graph G has a loop.

Our presentation of the previous results is essentially the same as that in [GJSW]. However, in that paper the authors claim in Proposition 1 that the analogue of 4.1.6 is true for completions of partial positive semidefinite matrices, but that is not entirely true. Here is a counterexample. Let G and A be as follows:

$$G = \begin{bmatrix} 1 & & & \\ & & & \\ & & & \\ 1 & 0 & x \end{bmatrix}$$

and $A = \begin{bmatrix} 1 & 0 & x \\ 0 & 0 & 1 \\ \overline{x} & 1 & y \end{bmatrix}$, where x and y denote unspecified entries.

Then A is a G-partial positive semidefinite matrix, $L = \{1, 2\}$, and the graph on L induced by G is complete, hence positive semidefinite completable. But A cannot be completed to a positive semidefinite matrix.

4.2 Extension of Banded Matrices

4.2.1 <u>Definition</u>. A k-banded matrix $A = [a_{ij}]$ satisfies $a_{ij} = 0$ whenever |i - j| > k. This means the middle 2k + 1 diagonal bands in A may have nonzero entries while the rest of A must be zero:

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1,k+1} & & \mathbf{0} \\ \vdots & \ddots & & \ddots & \\ a_{k+1,1} & & \ddots & & a_{n-k,n} \\ & \ddots & & \ddots & \vdots \\ \mathbf{0} & & a_{n,n-k} & \cdots & a_{nn} \end{bmatrix}.$$

4.2.2 <u>Definitions.</u> A lower corner k-banded matrix $A = [a_{ij}]$ satisfies $a_{ij} = 0$ whenever $i - j \le k$. This means the n - k - 1 diagonal bands in the lower left corner of A may have nonzero entries while the rest of A must be zero:

$$A = \begin{bmatrix} a_{k+2,1} & & & \\ \vdots & \ddots & & \\ a_{n1} & \cdots & a_{n,n-k-1} & \end{bmatrix}.$$

Similarly, an upper corner k-banded matrix $A = [a_{ij}]$ satisfies $a_{ij} = 0$ whenever $j - i \le k$. The n - k - 1 diagonal bands in the upper right corner of A may have nonzero entries while the rest of A must be zero:

$$A = \begin{bmatrix} a_{1,k+2} & \cdots & a_{1n} \\ & \ddots & \vdots \\ & & a_{n-k-1,n} \end{bmatrix}.$$

Assume henceforth that n and m, $0 \le m \le n - 1$, are fixed. Given an $n \times n$ matrix $R = [r_{ij}]$, R_L will denote the lower corner m-banded matrix whose diagonal bands in the lower left corner match those of R, entry for entry. That is, whenever i - j > m, the (i, j)-entry of R_L is r_{ij} , and the remaining entries of R_L are all zero. Similarly, R_U will denote the upper corner m-banded matrix whose diagonal bands in the upper right corner match those of R, entry for entry. In other words, whenever j - i > m, the (i, j)-entry of R_U is r_{ij} , and the remaining entries of R_U are all zero.

We say A admits a UDL factorization if there exist an upper triangular U, a diagonal D, and a lower triangular L such that the diagonal entries of U and L are all 1, and A = UDL.

- **4.2.3** <u>Definitions</u>. Given an m-banded matrix $A = [a_{ij}]$, an *extension* $F = [f_{ij}]$ of A is a matrix where $f_{ij} = a_{ij}$ whenever $|i j| \le m$. A *UDL extension* is an extension which admits a UDL factorization.
- **4.2.4** Notation. Given a matrix A, A(j,..., k) will denote the principal submatrix of A composed of rows and columns j through k. We sometimes refer to such submatrices as principal block submatrices.

4.2.5 Theorem. [DG] Let $R = [r_{ij}]$ be an m-banded matrix. Suppose all the following are nonsingular:

- (a) R(j,..., j + m), j = 1,..., n m (all (m+1)-by-(m+1) principal submatrices within the middle 2m + 1 diagonal bands of R),
- (b) R(j + 1,..., j + m), j = 1,..., n m 1 (all m-by-m principal block submatrices within the middle 2m + 1 diagonal bands of R, except the leading and the trailing),
- and (c) R(j,..., n), j = n m + 1,..., n (all trailing principal submatrices within the middle 2m + 1 diagonal bands of R of size $m \times m$ or smaller).

Then there exists a UDL extension F of R such that

$$F = (X_-VX_+)^{-1}$$
,

where X₋ is lower triangular and m-banded,

X, is upper triangular and m-banded,

V is diagonal and invertible,

and the diagonal entries of X₊ and X₋ are all 1.

Furthermore, given $\alpha = \alpha(j) = j + 1$ for j = 1,..., n - 1, and $\beta = \beta(j) = \min\{j + m, n\}$ for j = 1,..., n, the entries of X_- in the m bands below the diagonal (column by column) are

(4.2.6)
$$\begin{bmatrix} x_{\alpha j} \\ \vdots \\ x_{\beta j} \end{bmatrix} = -[R(\alpha, ..., \beta)]^{-1} \begin{bmatrix} r_{\alpha j} \\ \vdots \\ r_{\beta j} \end{bmatrix}$$
 for $j = 1, ..., n-1$;

similarly, the entries of X_+ in the m bands above the diagonal (row by row) are

(4.2.7)
$$[x_{j\alpha} \cdots x_{j\beta}] = -[r_{j\alpha} \cdots r_{j\beta}][R(\alpha,...,\beta)]^{-1}$$
 for $j = 1,..., n-1$;

and the diagonal entries of V are

(4.2.8)
$$\mathbf{v}_{jj} = ([\mathbf{R}(\mathbf{j},...,\boldsymbol{\beta})]^{-1})_{11}$$
 for $\mathbf{j} = 1,..., n$.

Proof. Define a lower triangular m-banded matrix $Z = [z_{ij}]$ as follows. Let $z_{ij} = 0$ if i < j or if i > j + m; further, for j = 1,..., n, define $\beta = \beta(j) = \min\{j + m, n\}$. Then $R(j,..., \beta)$ is invertible by hypothesis (a) or (c), and define column j of Z from the (j, j)-entry through the (β, j) -entry as

$$\begin{bmatrix} z_{jj} \\ \vdots \\ z_{\beta j} \end{bmatrix} = \left[R(j, ..., \beta) \right]^{-1} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

We claim that Z is invertible. Since $det(Z) = \prod_{j=1}^{n} z_{jj}$, if we can show each z_{jj} is nonzero, the

claim will follow immediately. For j = 1, we can block $R(1,...,\beta)\begin{bmatrix} z_{11} \\ \vdots \\ z_{\beta 1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ as

$$\begin{bmatrix} \mathbf{r}_{11} & \mathbf{r}_{12} \\ \mathbf{r}_{21} & \mathbf{R}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{z}_{11} \\ \mathbf{z}_{21} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

where
$$\vec{r}_{12} = \begin{bmatrix} r_{12} & \cdots & r_{1\beta} \end{bmatrix}$$
, $\vec{r}_{21} = \begin{bmatrix} r_{21} \\ \vdots \\ r_{\beta 1} \end{bmatrix}$, $\vec{R}_{22} = R(2,...,\beta)$, $\vec{z}_{21} = \begin{bmatrix} z_{21} \\ \vdots \\ z_{\beta 1} \end{bmatrix}$, and 0 is the

 $(\beta - 1) \times 1$ zero vector.

Hence
$$r_{11}z_{11} + r_{12}z_{21} = 1$$
 (1)

and
$$r'_{21}z_{11} + R'_{22}z'_{21} = 0.$$
 (2)

Since R'_{22} is nonsingular by hypothesis (b), equation (2) above is equivalent to

$$z'_{21} = -(R'_{22})^{-1}r'_{21}z_{11}.$$

Substituting this in (1) we get

$$\begin{split} & r_{11}z_{11} + r_{12}^{'} \left[-\left(R_{22}^{'}\right)^{-1}r_{21}^{'}z_{11} \right] = 1, \text{ i.e.,} \\ & \left[r_{11} - r_{12}^{'} \left(R_{22}^{'}\right)^{-1}r_{21}^{'} \right] z_{11} = 1 \text{ which implies } z_{11} \neq 0. \end{split}$$

Now for any j, we can block
$$R(j,\ldots,\beta)$$
 as $\begin{bmatrix} r_{jj} & r_{j2}'\\ r_{2j}' & R_{22}' \end{bmatrix}$

where
$$\mathbf{r}'_{j2} = \begin{bmatrix} \mathbf{r}_{j,j+1} & \cdots & \mathbf{r}_{j\beta} \end{bmatrix}$$
, $\mathbf{r}'_{2j} = \begin{bmatrix} \mathbf{r}_{j+1,j} \\ \vdots \\ \mathbf{r}_{\beta j} \end{bmatrix}$, and $\mathbf{R}'_{22} = \mathbf{R}(j+1,...,\beta)$.

Then
$$R(j,...,\beta)\begin{bmatrix} z_{jj} \\ \vdots \\ z_{\beta j} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$
 becomes $\begin{bmatrix} r_{jj} & r'_{j2} \\ r'_{2j} & R'_{22} \end{bmatrix} \begin{bmatrix} z_{jj} \\ z'_{2j} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$,

where
$$z'_{2j} = \begin{bmatrix} z_{j+1,j} \\ \vdots \\ z_{\beta j} \end{bmatrix}$$
 and 0 is the $(\beta - j) \times 1$ zero vector.

Reasoning as before, using hypothesis (b) or (c), we get

$$\mathbf{z}'_{2j} = -\left(\mathbf{R}'_{22}\right)^{-1} \mathbf{r}'_{2j} \mathbf{z}_{jj}$$

$$\begin{bmatrix} \mathbf{r} & \mathbf{r}' & \mathbf{R}' & \mathbf{r}' \\ \mathbf{r}' & \mathbf{r}' & \mathbf{r}' \end{bmatrix}_{\mathbf{r}} = 1 \text{ subjections}$$

and

$$\left[r_{jj} - r'_{j2} \left(R'_{22}\right)^{-1} r'_{2j}\right] z_{jj} = 1 \text{ which implies } z_{jj} \neq 0.$$

Thus we have shown that Z is nonsingular. In fact, we have shown a more general result:

For any
$$k \in \mathbb{N}$$
, if $\begin{bmatrix} z_1 \\ \vdots \\ z_k \end{bmatrix} = A \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$, and A and A(2,..., k) are nonsingular, then $z_1 \neq 0$. (*)

Now define an upper triangular m-banded matrix $W = [w_{ij}]$ as follows. Let $w_{ij} = 0$ if i > j or i < j - m; further, for i = 1, ..., n, define $\gamma = \gamma(i) = \min\{i + m, n\}$. Then $R(i, ..., \gamma)$ is invertible by hypothesis (a) or (c), and define row i of W from the (i, i)-entry through the (i, γ)-entry as

$$\begin{bmatrix} \mathbf{w}_{ii} & \cdots & \mathbf{w}_{i\gamma} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} \mathbf{R}(\mathbf{i}, \dots, \gamma) \end{bmatrix}^{-1}.$$

Then W is invertible since each $w_{ii} \neq 0$. To see this, note that

$$\begin{bmatrix} w_{ii} & \cdots & w_{i\gamma} \end{bmatrix}^t = \begin{bmatrix} \left[R(i, \dots, \gamma) \right]^{-1} \end{bmatrix}^t \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}^t, \text{ i.e.,}$$

$$\begin{bmatrix} w_{ii} \\ \vdots \\ w_{i\gamma} \end{bmatrix} = \begin{bmatrix} [R(i,...,\gamma)]^{-1} \end{bmatrix}^{t} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \text{ Thus by (*) above, } w_{ii} \neq 0.$$

Observe that $(RZ)_L Z^{-1}$ is a lower corner m-banded matrix. (This follows at once from the fact that $(RZ)_L$ is lower corner m-banded and Z^{-1} is lower triangular.) Similarly, $W^{-1}(WR)_U$ is an upper corner m-banded matrix.

Define an extension
$$F = [f_{ij}]$$
 of R by $F = F_L + R + F_U$,
where $F_L = -(RZ)_L Z^{-1}$ and $F_U = -W^{-1}(WR)_U$.

Note that $f_{ij} = r_{ij}$ when $|i - j| \le m$, as required for an extension. We will show that F admits a UDL factorization.

First note that $(F_UZ)_L = 0$ since F_U is upper corner m-banded and Z is lower triangular and m-banded. So

$$(FZ)_{L} = ((F_{L} + R + F_{U})Z)_{L} = (F_{L}Z + RZ + F_{U}Z)_{L}$$

$$= (F_{L}Z)_{L} + (RZ)_{L} + (F_{U}Z)_{L}$$

$$= (-(RZ)_{L}Z^{-1}Z)_{L} + (RZ)_{L} + 0$$

$$= (-(RZ)_{L})_{L} + (RZ)_{L}$$

$$= -(RZ)_{L} + (RZ)_{L}$$

$$= 0.$$

We also have

$$\begin{aligned} (WF)_{U} &= \left(W(F_{L} + R + F_{U})\right)_{U} = \left(WF_{L} + WR + WF_{U}\right)_{U} \\ &= \left(WF_{L}\right)_{U} + \left(WR\right)_{U} + \left(WF_{U}\right)_{U} \\ &= 0 + \left(WR\right)_{U} + \left(W(-W^{-1}(WR)_{U})\right)_{U} \\ &= \left(WR\right)_{U} + \left(-\left(WR\right)_{U}\right)_{U} \\ &= \left(WR\right)_{U} - \left(WR\right)_{U} \\ &= 0. \end{aligned}$$

We claim that FZ is upper triangular with 1's on the diagonal. Since $(FZ)_L = 0$, we need only show that the (i, j)-entry of FZ, $(FZ)_{ij}$, is zero whenever $j + 1 \le i \le \beta$, where $\beta = \min\{j + m, n\}$, i.e., FZ is zero in the diagonal bands below the main diagonal.

First note that for $j + 1 \le i \le \beta$,

$$\begin{aligned} (FZ)_{ij} &= \sum_{k=j}^{\beta} f_{ik} z_{kj} & \text{since Z is lower triangular m-banded} \\ &= \sum_{k=i}^{\beta} r_{ik} z_{kj} & \text{since } \left[f_{ij} & \cdots & f_{i\beta} \right] = \left[r_{ij} & \cdots & r_{i\beta} \right]. \end{aligned}$$

Recall that $R(j,...,\beta)\begin{bmatrix} z_{jj} \\ \vdots \\ z_{\beta j} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ for each j = 1,..., n (from how we defined Z), i.e.,

$$\begin{bmatrix} \mathbf{r}_{\mathbf{j}\mathbf{j}} & \cdots & \mathbf{r}_{\mathbf{j}\beta} \\ \vdots & \ddots & \vdots \\ \mathbf{r}_{\beta\mathbf{j}} & \cdots & \mathbf{r}_{\beta\beta} \end{bmatrix} \begin{bmatrix} \mathbf{z}_{\mathbf{j}\mathbf{j}} \\ \vdots \\ \mathbf{z}_{\beta\mathbf{j}} \end{bmatrix} = \begin{bmatrix} \mathbf{1} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix}.$$

Hence for each j=1,...,n, we have $1=r_{ij}z_{jj}+\cdots+r_{j\beta}z_{\beta j}=\sum_{k=j}^{\beta}r_{jk}z_{kj}=(FZ)_{jj}$ from above;

thus we have shown that each diagonal entry of FZ is 1.

In addition, for each j = 1,..., n - 1, we have

$$0 = r_{j+1,j} z_{jj} + r_{j+1,j+1} z_{j+1,j} + \dots + r_{j+1,\beta} z_{\beta j} = \sum_{k=j}^{\beta} r_{j+1,k} z_{kj} = (FZ)_{j+1,j} \text{ from above.}$$

Thus $(FZ)_{ij} = 0$ when i - j = 1.

Similarly, for each j = 1,..., n - 2, we have

$$0 = r_{j+2,j} z_{jj} + r_{j+2,j+1} z_{j+1,j} + \dots + r_{j+2,\beta} z_{\beta j} = \sum_{k=j}^{\beta} r_{j+2,k} z_{kj} = (FZ)_{j+2,j} \text{ from above.}$$

Hence $(FZ)_{ij} = 0$ when i - j = 2.

Continuing in the same way, it follows that $(FZ)_{ij} = 0$ whenever $1 \le i - j \le m$ which, together with $(FZ)_L = 0$, imply that FZ is upper triangular.

A similar argument can be applied to show that WF is lower triangular with 1's on the diagonal; we supply the following details. Since $(WF)_U = 0$, we only need to show that $(WF)_{ij} = 0$ whenever $i + 1 \le j \le \gamma$, where $\gamma = \min\{i + m, n\}$, i.e., WF is zero in the diagonal bands above the main diagonal.

For $i + 1 \le j \le \gamma$, we have

$$(WF)_{ij} = \sum_{k=i}^{\gamma} w_{ik} f_{kj} \quad \text{since W is upper triangular m-banded}$$

$$= \sum_{k=i}^{\gamma} w_{ik} r_{kj} \quad \text{since } \left[f_{ij} \quad \cdots \quad f_{ij} \right] = \left[r_{ij} \quad \cdots \quad r_{ij} \right].$$

Recall that $\begin{bmatrix} w_{ii} & \cdots & w_{i\gamma} \end{bmatrix} R(i,...,\gamma) = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}$ for each i=1,...,n (from how we defined W), i.e.,

$$\begin{bmatrix} \mathbf{w}_{ii} & \cdots & \mathbf{w}_{i\gamma} \end{bmatrix} \begin{bmatrix} \mathbf{r}_{ii} & \cdots & \mathbf{r}_{i\gamma} \\ \vdots & \ddots & \vdots \\ \mathbf{r}_{\gamma i} & \cdots & \mathbf{r}_{\gamma \gamma} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}.$$

Hence for each i = 1, ..., n, we have

$$1 = w_{ii}r_{ii} + \dots + w_{i\gamma}r_{\gamma i} = \sum_{k=i}^{\gamma} w_{ik}r_{ki} = (WF)_{ii} \text{ from above;}$$

so every diagonal entry of WF is 1.

In addition, for each i = 1, ..., n - 1, we have

$$0 = w_{ii}r_{i,i+1} + w_{i,i+1}r_{i+1,i+1} + \dots + w_{i\gamma}r_{\gamma,i+1} = \sum_{k=i}^{\gamma} w_{ik}r_{k,i+1} = (WF)_{i,i+1} \text{ from above.}$$

Thus $(WF)_{ij} = 0$ when j - i = 1.

Similarly, for each i = 1, ..., n - 2, we have

$$0 = w_{ii}r_{i,i+2} + w_{i,i+1}r_{i+1,i+2} + \dots + w_{i\gamma}r_{\gamma,i+2} = \sum_{k=i}^{\gamma} w_{ik}r_{k,i+2} = (WF)_{i,i+2} \text{ from above.}$$

Hence $(WF)_{ij} = 0$ when j - i = 2.

Continuing in the same way, it follows that $(WF)_{ij} = 0$ whenever $1 \le j - i \le m$ which, together with $(WF)_{ij} = 0$, imply that WF is lower triangular.

Let U = FZ and L = WF. Then U and L are invertible since each has only 1's on its diagonal, and LZ = WFZ = WU. Since L and Z are both lower triangular, so is LZ; also since W and U are both upper triangular, so is WU. Therefore, LZ = WFZ = WU is diagonal and also invertible since L and Z are both invertible. Furthermore,

$$F = W^{-1}(WU)Z^{-1}$$

is invertible and

$$F^{-1} = Z(WU)^{-1}W$$
$$= X_{-}VX_{+},$$

where

 $X_{-} = Zdiag(1/z_{11},..., 1/z_{nn})$ is lower triangular m-banded with 1's on the diagonal,

 $X_{+} = diag(1/w_{11},..., 1/w_{nn})W$ is upper triangular m-banded with 1's on the diagonal, and $V = diag(z_{11},...,z_{nn})(WU)^{-1}diag(w_{11},...,w_{nn})$ is diagonal and invertible.

To complete the proof, we verify the formulas (4.2.6) - (4.2.8). First note that $F = (X_-VX_+)^{-1}$ implies $FX_-V = (X_+)^{-1}$. Writing out the jth column of this identity from the (j, j)-entry through the (β, j) -entry, we get

(**)
$$F(j,...,\beta)\begin{bmatrix} x_{jj} \\ \vdots \\ x_{\beta j} \end{bmatrix} v_{jj} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \text{ where } \beta = \beta(j) = \min\{j+m, n\} \text{ and } x_{kj} \text{ is the } (k, j)\text{-entry}$$

of X₋. The right-hand side in (**) follows because X₊ is upper triangular with 1's on the diagonal; hence $(X_+)^{-1}$ must have the same properties. Since F is an extension of R and $\beta - j \le m$, $F(j, ..., \beta) = R(j, ..., \beta)$; thus

$$\begin{bmatrix} x_{jj} \\ \vdots \\ x_{\beta j} \end{bmatrix} v_{jj} = [R(j,...,\beta)]^{-1} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Then since $x_{jj} = 1$, it follows that v_{jj} is the (1, 1)-entry of $[R(j,...,\beta)]^{-1}$ which proves (4.2.8).

Since V is invertible and diagonal, its diagonal entries must all be nonzero; hence (**) also implies

$$\begin{bmatrix} f_{\alpha j} & \cdots & f_{\alpha \beta} \\ \vdots & \ddots & \vdots \\ f_{\beta j} & \cdots & f_{\beta \beta} \end{bmatrix} \begin{bmatrix} x_{jj} \\ \vdots \\ x_{\beta j} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \text{ for } j = 1, \dots, n-1 \text{ where } \alpha = \alpha(j) = j+1.$$

Then since $x_{ii} = 1$, we have

$$0 = f_{\alpha j} + f_{\alpha \alpha} x_{\alpha j} + \dots + f_{\alpha \beta} x_{\beta j}$$

= $r_{\alpha j} + r_{\alpha \alpha} x_{\alpha j} + \dots + r_{\alpha \beta} x_{\beta j}$ since F is an extension of R and $\beta - \alpha \le m$.

Thus
$$\begin{bmatrix} r_{\alpha\alpha} & \cdots & r_{\alpha\beta} \end{bmatrix} \begin{bmatrix} x_{\alpha j} \\ \vdots \\ x_{\beta j} \end{bmatrix} = -r_{\alpha j}$$
.

Similarly, for $k \in \{\alpha, ..., \beta\}$, we have

$$0 = f_{kj} + f_{k\alpha} x_{\alpha j} + \dots + f_{k\beta} x_{\beta j}$$

$$= r_{kj} + r_{k\alpha} x_{\alpha j} + \cdots + r_{k\beta} x_{\beta j}.$$

Thus
$$\begin{bmatrix} r_{k\alpha} & \cdots & r_{k\beta} \end{bmatrix} \begin{bmatrix} x_{\alpha j} \\ \vdots \\ x_{\beta j} \end{bmatrix} = -r_{kj}$$
 for each $k \in \{\alpha, ..., \beta\}$ and $j = 1, ..., n-1$.

Hence
$$R(\alpha,...,\beta)\begin{bmatrix} x_{\alpha j} \\ \vdots \\ x_{\beta j} \end{bmatrix} = -\begin{bmatrix} r_{\alpha j} \\ \vdots \\ r_{\beta j} \end{bmatrix}$$
 for each $j=1,...,n-1$ which is equivalent to (4.2.6).

Finally, a similar argument can be applied to verify (4.2.7); we supply the following details. First note that $F = (X_-VX_+)^{-1}$ implies $VX_+F = (X_-)^{-1}$. Writing out the jth row of this identity from the (j, j)-entry through the (j, β) -entry, we get

(***)
$$v_{jj}[x_{jj} \cdots x_{j\beta}]F(j,...,\beta) = [1 \ 0 \ \cdots \ 0],$$

where $\beta = \beta(j) = \min\{j + m, n\}$ and x_{jk} is the (j, k)-entry of X_{+} . The right-hand side in (***) follows because X_{-} is lower triangular with 1's on the diagonal; hence $(X_{-})^{-1}$ has the same properties. Since the diagonal entries of V are nonzero, (***) implies

$$\begin{bmatrix} x_{jj} & \cdots & x_{j\beta} \end{bmatrix} \begin{bmatrix} f_{j\alpha} & \cdots & f_{j\beta} \\ \vdots & \ddots & \vdots \\ f_{\beta\alpha} & \cdots & f_{\beta\beta} \end{bmatrix} = \begin{bmatrix} 0 & \cdots & 0 \end{bmatrix} \text{ for } j = 1, \dots, n-1 \text{ where } \alpha = \alpha(j) = j+1.$$

For $k \in \{\alpha, ..., \beta\}$, we have

$$0 = f_{ik} + x_{i\alpha}f_{\alpha k} + \cdots + x_{i\beta}f_{\beta k} \text{ since } x_{ij} = 1$$

= $r_{jk} + x_{j\alpha}r_{\alpha k} + \cdots + x_{j\beta}r_{\beta k}$ since F is an extension of R and β - $\alpha \le m$.

Thus
$$-r_{jk} = \begin{bmatrix} x_{j\alpha} & \cdots & x_{j\beta} \end{bmatrix} \begin{bmatrix} r_{\alpha k} \\ \vdots \\ r_{\beta k} \end{bmatrix}$$
 for each $k \in \{\alpha, ..., \beta\}$ and $j = 1, ..., n-1$.

Hence $-[r_{j\alpha} \cdots r_{j\beta}] = [x_{j\alpha} \cdots x_{j\beta}]R(\alpha,...,\beta)$ for each j = 1,..., n-1 which is equivalent to (4.2.7).

- **4.2.9** Theorem. [DG] Let $R = [r_{ij}]$ be an m-banded matrix. Then the following are equivalent:
 - (1) R admits a positive definite UDL extension F.
- (2) Each of the principal submatrices R(j,...,j+m), j=1,...,n-m, is positive definite. (That is, any principal (m+1)-by-(m+1) submatrix contained within the middle 2m+1 diagonal bands of R is positive definite.)

Proof. (1) \Rightarrow (2) Suppose R admits a positive definite UDL extension F. Then for each j = 1, ..., n - m, R(j, ..., j + m) = F(j, ..., j + m) which is positive definite since it is a principal submatrix of the positive definite F.

 $(2) \Rightarrow (1)$ Suppose for each j = 1, ..., n - m, R(j, ..., j + m) is positive definite. Then each principal submatrix of each R(j, ..., j + m) is positive definite, hence nonsingular. Thus conditions (a), (b), and (c) of Theorem 4.2.5 are satisfied, and so there exists a UDL extension F of R with $F^{-1} = X_-VX_+$, where X_- , X_+ and V are as described in Theorem 4.2.5. We will show that F^{-1} is positive definite which implies that F is.

To see that F^{-1} is Hermitian, let $\alpha = \alpha(j) = j + 1$ for j = 1, ..., n - 1, and $\beta = \beta(j) = \min\{j + m, n\}$ for j = 1, ..., n. Then for each j = 1, ..., n - 1, $R(\alpha, ..., \beta)$ is one of the matrices assumed to be positive definite or is a principal submatrix of one of these matrices. Hence $R(\alpha, ..., \beta)$ is positive definite which implies $[R(\alpha, ..., \beta)]^{-1}$ is positive definite. Also by assumption, R is Hermitian within its middle 2m + 1 diagonal bands, i.e., $\overline{r_{kj}} = r_{jk}$ for every $k \in \{\alpha, ..., \beta\}$ and every $j \in \{1, ..., n - 1\}$. Thus we have for each j = 1, ..., n - 1,

$$\begin{bmatrix} x_{\alpha j} \\ \vdots \\ x_{\beta j} \end{bmatrix}^* = -\begin{bmatrix} \overline{r_{\alpha j}} & \cdots & \overline{r_{\beta j}} \end{bmatrix} ([R(\alpha, ..., \beta)]^{-1})^* \quad \text{by (4.2.6)}$$

$$= -[r_{j\alpha} & \cdots & r_{j\beta}][R(\alpha, ..., \beta)]^{-1} \quad \text{from above}$$

$$= [x_{j\alpha} & \cdots & x_{j\beta}] \quad \text{by (4.2.7)}.$$

Therefore $X_{-}^* = X_{+}$ and so $X_{+}^* = X_{-}$. Now we have

$$(F^{-1})^* = (X_-VX_+)^* = X_+^*V^*X_-^*$$

= X_-VX_+ from above
= F^{-1} .

Hence F-1 is Hermitian.

To see that F^{-1} is positive definite, we first show that V is positive definite. For each $j = 1,..., n, R(j,..., \beta)$ is one of the matrices assumed to be positive definite or is a principal submatrix of one of these matrices. Hence $R(j,..., \beta)$ is positive definite which implies $[R(j,..., \beta)]^{-1}$ is positive definite. Thus each diagonal entry of $[R(j,..., \beta)]^{-1}$ is positive which implies each diagonal entry of V must be positive by (4.2.8). Hence since V is diagonal, V is positive definite.

Now let $y \neq \theta$. Since X_+ is nonsingular, $x = X_+y \neq \theta$. So

$$y^*F^{-1}y = y^*X_-VX_+y$$
$$= x^*Vx$$

> 0 since V is positive definite.

Thus F-1 is positive definite which implies F is positive definite.

Notice the preceding theorem can be restated in terms of partial matrices.

- **4.2.10** Corollary. [GJSW] Fix an integer m, $0 \le m \le n 1$. Suppose $A = [a_{ij}]$ is a partial matrix in which a_{ij} is specified if and only if $|i j| \le m$ (i.e., just the middle 2m + 1 diagonal bands in A are specified). Then the following are equivalent:
- (1) There exists a positive definite completion of A, i.e.,
 {B: B is positive definite and b_{ij} = a_{ij} for all |i j| ≤ m} ≠ Ø.
- (2) Any principal (m + 1)-by-(m + 1) submatrix contained within the middle 2m + 1 diagonal bands of A is positive definite (i.e., any completely specified (m + 1)-by-(m + 1) principal submatrix of A is positive definite).

Note that (2) is equivalent to

(2') Every completely specified principal submatrix of A is positive definite.

4.3 Band Graphs

- **4.3.1** <u>Definitions</u>. Given a graph G = (V, E), an *ordering* of V is a bijection $\sigma: \{1, 2, ..., n\} \rightarrow V$. We sometimes indicate an ordering by using the notation $V = \{x_i\}_{i=1}^n$. If V is ordered by σ , then $G_{\sigma} = (V, E, \sigma)$ is an *ordered graph* associated with G.
- **4.3.2** Definition. A graph G = (V, E) is called a band graph if there exists an ordering σ of V and an integer m, $0 \le m \le n 1$, such that $\{x, y\} \in E$ if and only if $|\sigma^{-1}(x) \sigma^{-1}(y)| \le m$.

Notice that if G is a band graph as above, then any G-partial matrix has just its middle 2m + 1 diagonal bands specified. Hence we have the following:

4.3.3 Corollary. [GJSW] If G is a band graph, then G is completable. Proof. Suppose G is a band graph and let A(G) be a G-partial positive definite matrix. Then every completely specified principal submatrix of A(G) is positive definite, i.e., (2) holds in Corollary 4.2.10. Thus by Corollary 4.2.10, A(G) has a positive definite completion which implies G is completable.

4.4 Perfect Elimination Orderings and Chordality

- **4.4.1** <u>Definitions.</u> Given a graph G = (V, E) and a vertex $x \in V$, the set $Adj(x) = \{y \in V: \{x, y\} \in E\}$ is the set of vertices *adjacent* to x. For distinct vertices $x, y \in V$, a *chain* from x to y (of length m) is an ordered set of distinct vertices $\mu = [p_1, p_2, ..., p_{m+1}]$ where $p_1 = x$ and $p_{m+1} = y$, such that $p_{i+1} \in Adj(p_i)$ for i = 1, ..., m. Similarly, a *cycle* (of length m) is an ordered set $\mu = [p_1, p_2, ..., p_m, p_1]$ such that $[p_1, ..., p_m]$ is a chain and $p_1 \in Adj(p_m)$. A graph G is *connected* if for each pair of distinct vertices $x, y \in V$, there is a chain from x to y.
- **4.4.2 Definition.** A graph G is *chordal* if for every cycle $\mu = [p_1, ..., p_m, p_1]$ of length $m \ge 4$, there is an edge of G joining two nonconsecutive vertices of μ ; such an edge is called a *chord* of the cycle.

Chordal graphs have also been called *triangulated* in [Ros] and [LRT].

The main result of this chapter will be proved in section 4.5 and says that if G is a graph which contains all possible loops, then G is completable if and only if G is chordal. Notice that this is an extension of Corollary 4.3.3 since band graphs are chordal.

To prove this major result requires a good deal of preliminary work which we outline here. It turns out that given any chordal graph G, it is possible to add one edge at a time to get a sequence of chordal graphs culminating with the complete graph. Given any G-partial positive definite matrix, this sequence of chordal graphs provides an order for specifying entries in the matrix so we end up with a positive definite completion.

However, it is also possible to add edges so that one of the graphs in the sequence is not chordal. Therefore, it is necessary to add edges carefully to get a sequence of chordal graphs. In section 4.7, we provide an algorithm for doing this which relies on a special

ordering of the vertices called a perfect elimination ordering. It turns out that a graph has a perfect elimination ordering if and only if it is chordal, which provides the foundation for proving that the sequence of chordal graphs exists. The remainder of this section is devoted to establishing the perfect elimination ordering-chordal equivalence.

4.4.3 Definitions. A separator of a connected graph G = (V, E) is a subset S of V such that the induced subgraph G(V - S) consists of two or more disjoint connected subgraphs of G, say $C_i = (V_i, E_i)$. We will call such C_i components of G(V - S). The leaves of G with respect to G are the induced subgraphs $G(S \cup V_i)$. A minimal separator is a separator no subset of which is also a separator. Given G with G with G and G with G and G such that G and G and G such that G such that G and G such that G is a subset G such that G such that G is a subset G

Note that a minimal separator is a minimal a, b separator for some a, $b \in V$, but a minimal a, b separator is not, in general, a minimal separator.

4.4.4 Definitions. Given an ordered graph $G_{\sigma} = (V, E, \sigma)$ and a vertex $x \in V$, the set of vertices monotonely adjacent to x is MAdj(x) = Adj(x) $\cap \{z \in V: \sigma^{-1}(z) > \sigma^{-1}(x)\}$. The deficiency of x, D(x), is the set of all pairs from Adj(x) which are not themselves adjacent, i.e., D(x) = $\{\{y, z\}: y, z \in Adj(x) \text{ and } y \notin Adj(z)\}$. Note that D(x) is a set of edges missing from G. Similarly, the monotone deficiency of x, MD(x), is the set MD(x) = $\{\{y, z\}: y, z \in MAdj(x) \text{ and } y \notin Adj(z)\}$. Note that MD(x) $\subseteq D(x)$.

- **4.4.5** Definition. Given a vertex y of a graph G = (V, E), the graph G_y obtained from G by
 - (1) deleting y and its incident edges
- and (2) adding edges so that all vertices in the set Adj(y) are adjacent to each other is the y-elimination graph of G. Thus

$$G_y = (V - \{y\}, E(V - \{y\}) \cup D(y)).$$

4.4.6 Lemma. If G is connected, then G_y is connected.

Proof. Let $x, w \in V - \{y\}$. Then there is a chain $[x, v_1, \ldots, v_k, w]$ in G which either contains y or does not. (Case 1) If the chain does not contain y, then $v_i \neq y$ for $i = 1, \ldots, k$, and so $[x, v_1, \ldots, v_k, w]$ is also a chain in G_y . (Case 2) If the chain contains y, then $y = v_j$ for some $j \in \{1, \ldots, k\}$; and because $v_{j-1}, v_{j+1} \in Adj(y), \{v_{j-1}, v_{j+1}\}$ is an edge in G_y . Thus $[x, \ldots, v_{j-1}, v_{j+1}, \ldots, w]$ is a chain in G_y . Hence in each case, we have shown that G_y contains a chain from x to w. Therefore, since x and y were chosen arbitrarily, y is connected.

4.4.7 Definition. For an ordered graph $G_{\sigma} = (V, E, \sigma)$,

the order sequence of elimination graphs $G_1, \ldots, G_{n\text{-}1}$ is defined recursively by

$$G_1 = G_{x_1}$$
 and

$$G_i = (G_{i-1})_{x_i}$$
 for $i = 2,..., n-1$.

4.4.8 <u>Definitions.</u> The *elimination process* on an ordered graph $G_{\sigma} = (V, E, \sigma)$ is the ordered set $[G_{\sigma} = G_0, G_1, ..., G_{n-1}]$. An elimination process is *perfect* if $G_i = G_0 \left(V - \bigcup_{j=1}^i \{x_j\} \right)$ for i = 1, ..., n - 1. In such a case, we will also refer to σ as a

perfect elimination ordering.

It may be helpful at this point to quickly review the various notations on G that we have introduced:

- G_{σ} is a graph whose vertices are ordered by σ
- G_{x_k} is the x_k -elimination graph of G; see 4.4.5
- G_i is the ith element of the order sequence of elimination graphs for G_{σ} ; see 4.4.7. Note that $G_i = G_{x_i}$ when i = 1 but not otherwise.

The following lemma brings together observations from [LRT] and [Ros].

- **4.4.9** Lemma. Given an ordered graph $G_{\sigma} = (V, E, \sigma)$, the following are equivalent:
 - (1) σ is a perfect elimination ordering.
 - (2) $D(x_i) = \emptyset$ in G_{i-1} for i = 1,..., n-1.
 - (3) $MD(x) = \emptyset$ for each $x \in V$.
- (4) For each $x \in V$, if $w, z \in MAdj(x)$, then $w \in Adj(z)$ or w = z. This will be called the *monotone transitive property*, and any graph with this property will be called *monotone transitive*.

Proof. (1) \Rightarrow (2) Suppose σ is a perfect elimination ordering. Then $G_{x_1} = G_1 = G_0(V - \{x_1\})$.

But by definition, $G_{x_1} = (V - \{x_1\}, E(V - \{x_1\}) \cup D(x_1))$ which means $D(x_1) = \emptyset$ in G_0 . Similarly, $G_i = G_0 \left(V - \bigcup_{j=1}^i \{x_j\} \right)$ for i = 1, ..., n-1. But $G_i = \left(G_{i-1} \right)_{x_i}$ by definition, which equals $\left(G_0 \left(V - \bigcup_{j=1}^{i-1} \{x_j\} \right) \right)_{x_i}$ since σ is perfect. But again by definition, this is just $\left(V - \bigcup_{j=1}^i \{x_j\}, E \left(V - \bigcup_{j=1}^i \{x_j\} \right) \cup D(x_i) \right)$ where $D(x_i)$ denotes the deficiency of x_i in G_{i-1} .

Thus, for i = 1,..., n - 1, we have $G_i = G_0 \left(V - \bigcup_{j=1}^i \{x_j\} \right) = \left(V - \bigcup_{j=1}^i \{x_j\}, \ E \left(V - \bigcup_{j=1}^i \{x_j\} \right) \cup D(x_i) \right) \text{ which implies that } D(x_i) = \emptyset \text{ in } G_{i-1}.$

- (2) \Rightarrow (3) Suppose $D(x_i) = \emptyset$ in G_{i-1} for i = 1, ..., n-1, and let $v \in V$. If v is x_n , then by its definition, MD(v) is empty. Otherwise, $v = x_j$ for some $j \in \{1, ..., n-1\}$; and since $MD(x_j) = D(x_j)$ in G_{i-1} , $MD(v) = MD(x_j) = \emptyset$.
- (3) \Rightarrow (4) Suppose MD(v) = \varnothing for each $v \in V$. Let $x \in V$ and $w, z \in MAdj(x)$. Then since MD(x) = \varnothing , $w \in Adj(z)$ or w = z by the definition of monotone deficiency.
- $(4) \Rightarrow (1) \text{ Suppose for each } x \in V, \text{ if } w, z \in MAdj(x), \text{ then } w \in Adj(z) \text{ or } w = z.$ We use induction to show σ is a perfect elimination ordering. First, by our assumption and the definition of monotone deficiency, $MD(x_1) = \emptyset$. Then since $MD(x_i) = D(x_i)$ in G_{i-1} , we have $D(x_1) = \emptyset$ in G_0 . Thus $G_1 \equiv \left(V \{x_1\}, \ E(V \{x_1\}) \cup D(x_1)\right) = G_0\left(V \{x_1\}\right)$.

Let k-1 be a positive integer less than n-1 such that $G_i = G_0 \left(V - \bigcup_{j=1}^i \{x_j\} \right)$ for $i=1,\ldots,k-1$. Then $G_k \equiv \left(G_{k-1} \right)_{x_k} = \left(G_0 \left(V - \bigcup_{j=1}^{k-1} \{x_j\} \right) \right)_{x_k}$ by the inductive hypothesis, which, by definition, equals $\left(V - \bigcup_{j=1}^k \{x_j\}, \ E \left(V - \bigcup_{j=1}^k \{x_j\} \right) \cup D(x_k) \right)$ where $D(x_k)$ denotes

deficiency, $MD(x_k) = \emptyset$ which implies that $D(x_k) = \emptyset$ in G_{k-1} . Hence $G_k = G_0\bigg(V - \bigcup_{j=1}^k \{x_j\}\bigg).$ Thus we have shown that $G_i = G_0\bigg(V - \bigcup_{j=1}^i \{x_j\}\bigg)$ for $i=1,\ldots,n-1$,

the deficiency of x_k in G_{k-1} . But by our assumption and the definition of monotone

i.e., σ is a perfect elimination ordering.

Recall that our immediate goal is to show that a graph G has a perfect elimination ordering if and only if G is chordal. The following theorem together with Lemma 4.4.9 establish this for a connected graph.

- **4.4.10** Theorem. [Ros] For a connected graph G = (V, E), the following statements are equivalent:
 - (1) There exists an ordering σ of V such that $G_{\sigma} = (V, E, \sigma)$ is monotone transitive.
 - (2) The graph G is chordal.
 - (3) For each a, b ∈ V with a ∉ Adj(b), every minimal a, b separator of G is a clique.

We will prove Theorem 4.4.10 in stages, using a series of lemmas.

4.4.11 Lemma. [Ros] A monotone transitive graph is chordal.

Proof. Let G_{σ} be a monotone transitive graph and let μ be any cycle of length $\ell \geq 4$. Let $p^* \in \mu$ be the vertex such that $\sigma^{-1}(p^*) = \min_{p \in \mu} \sigma^{-1}(p)$. Since p^* is adjacent to two nonconsecutive vertices in the cycle μ (because $\ell \geq 4$), and σ^{-1} maps each of these to integers greater than $\sigma^{-1}(p^*)$, both are in MAdj(p^*). Since G_{σ} is monotone transitive, these two vertices must be adjacent to one another which means μ has a chord.

4.4.12 Lemma. [Ros] In a connected chordal graph G = (V, E), for each $a, b \in V$ with $a \notin Adj(b)$, every minimal a, b separator of G is a clique.

Proof. Let G = (V, E) be connected and chordal, and let $a, b \in V$ with $a \notin Adj(b)$. Let S be a minimal a, b separator of G, and let C_a and C_b be the components of G(V - S) containing a and b, respectively. If |S| = 1, we are done. (Recall we have assumed that our graphs contain all possible loops.) Otherwise, since S is minimal, each $q \in S$ is adjacent to some vertex in C_a and some vertex in C_b . (For if not, then S - q would be an a, b separator of G.) Let $x, y \in S$ and let μ_1 be a shortest chain of the type $\left[x, c_{11}, c_{12}, \ldots, c_{1,p_1}, y\right]$ where each $c_{1i} \in C_a$ and $c_{1i} \in C_a$

 $\begin{bmatrix} x, \ c_{21}, \ c_{22}, ..., \ c_{2,p_2}, \ y \end{bmatrix}$ where each $c_{2i} \in C_b$ and $p_2 \ge 1$. The cycle $\begin{bmatrix} x, \ c_{11}, ..., \ c_{1,p_1}, \ y, \ c_{2,p_2}, ..., \ c_{2l}, \ x \end{bmatrix}$ has length ≥ 4 and the only possible chord is $\{x, y\}$ since μ_1 and μ_2 were chosen to be shortest. Since x and y were chosen arbitrarily, we have shown that S is a clique.

The following three lemmas build one on the next and culminate in establishing the integral part of proving $(3) \Rightarrow (1)$ in Theorem 4.4.10. It appears necessary to involve significant insight and a good number of steps to prove that a graph has a perfect elimination ordering when starting without an ordering. While it may not be clear from their statements that the lemmas build one on the next, the proofs will demonstrate that they do in small but significant ways.

4.4.13 Lemma. [Ros] Let G = (V, E) be a connected graph with separation clique S. Let $G(V-S) = \bigcup_{i=1}^{m} C_i$ where $m \ge 2$, $C_i = (V_i, E_i)$ is the ith component of G(V-S), $V_i \cap V_j = \emptyset$ for $i \ne j$, and no two vertices in different components are adjacent to each

 $V_i \cap V_j = \emptyset$ for $i \neq j$, and no two vertices in different components are adjacent to each other. Let $L_i = G(S \cup V_i)$ be the leaves of G with respect to S.

- (i) Let S_0 be a separator of an L_r for some $r \in \{1,..., m\}$. Then S_0 is a separator of G.
- (ii) Furthermore, if a, b ∈ L_T with a ∉ Adj(b), and S₀ is a minimal a, b separator of
 L_T, then S₀ is a minimal a, b separator of G.

Proof of (i). Suppose S_0 is a separator of an L_r for some $r \in \{1,..., m\}$. Then $S_0 \subset S \cup V_r$. Let D_j , j = 1,..., p, be the components of $L_r((S \cup V_r) - S_0)$. Since the vertices of S are among those of L_r , and S is a clique, the vertices of S must all be in $S_0 \cup V(D_k)$ for some fixed $k \in \{1,...,p\}$, where $V(D_k)$ denotes the vertices of D_k .

Since $p \ge 2$, let $x \in V(D_k)$ and let $y \in V(D_t)$, $t \ne k$. We claim that any chain from y to x must contain a vertex of S_0 . Any chain from y to x which leaves L_T contains a vertex of S because $y \in V_T$ and S separates V_T from the other vertices of G. Consider the part of such a chain from y to S and lying in L_T . Since $S \subseteq S_0 \cup V(D_k)$, the chain must contain a vertex of S_0 or a vertex of $V(D_k)$. In either case, because S_0 separates y from $V(D_k)$ in L_T , the chain must include a vertex of S_0 . Thus we have shown that any chain from y to x which leaves L_T contains a vertex of S_0 . And since any chain from y to x lying in L_T contains a vertex of S_0 , we conclude that any chain from y to x includes a vertex of S_0 . This implies that $G(V - S_0)$ is not connected, i.e., S_0 is a separator of G.

Proof of (ii). Suppose $a, b \in L_r$ for some $r \in \{1,..., m\}$ with $a \notin Adj(b)$, and suppose that S_0 is a minimal a, b separator of L_r . Let D_j be defined as in part (i) and suppose $a \in V(D_1)$ and $b \in V(D_2)$. Since $S \subseteq S_0 \cup V(D_k)$ for some fixed $k \in \{1,..., p\}$, and $p \ge 2$, we may assume that $k \ne 2$.

We claim that S_0 is an a, b separator of G. Consider any chain in G from a to b. We will show that it includes a vertex of S_0 . If the chain lies entirely in L_r , then it must contain a vertex of S_0 because S_0 separates a from b in L_r . Otherwise, some vertex of the chain is not in L_r . Then by the argument from part (i), the chain must contain a vertex of S_0 . Thus we have shown that any chain in G from a to b includes a vertex of S_0 which implies S_0 is an a, b separator of G.

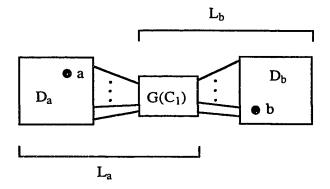
Finally S_0 is a minimal a, b separator of G since any a, b separator $S_1 \subset S_0$ of G is an a, b separator of L_T , and S_0 is a minimal such separator of L_T .

4.4.14 Lemma. [Ros] Let G = (V, E) be a connected graph such that for each a, b ∈ V with a ∉ Adj(b), every minimal a, b separator of G is a clique. (4.4.15)

Then either V is a clique or given any clique $C \subset V$, there exists a vertex $x \notin C$ such that $D(x) = \emptyset$ (in G).

Proof. The proof is by induction on the number of vertices, |V|, and the case |V| = 1 is clear. Suppose the Lemma is true for a graph which has at most k vertices. Let G = (V, E) be a graph with k + 1 vertices which satisfies the hypotheses of the Lemma, and let C be any clique in G. (A clique will always exist because G contains all possible loops.) We need to prove that V is a clique or there exists a vertex $x \notin C$ such that $D(x) = \emptyset$ in G.

Suppose V is not a clique. Let $a, b \in V$ with $a \notin Adj(b)$. Let C_1 be a minimal a, b separator of G. Then by (4.4.15), C_1 is a clique. Let D_a , D_b and L_a , L_b be the corresponding components of $G(V - C_1)$ and leaves of G with respect to C_1 containing a and b, respectively. Since C is a clique, the vertices of $C - C_1$ (if any) can be in at most one component of $G(V - C_1)$. Suppose such vertices are <u>not</u> in $V(D_b)$, where $V(D_b)$ denotes the vertices of D_b (see picture).



Let W be the set of vertices of L_b . Then $|W| \le k$ because $a \in V(D_a)$ which implies $a \notin V(L_b)$. We claim that L_b satisfies the hypotheses of this Lemma. It is connected because $W = C_1 \cup V(D_b)$, D_b is connected, and each vertex in C_1 is adjacent to a vertex in D_b since C_1 is minimal. Also for each c, $d \in V(L_b)$ with $c \notin Adj(d)$, any minimal c, d separator of L_b is a clique because it is also a minimal c, d separator of G by Lemma 4.4.13(ii), hence is a clique by (4.4.15). Thus we have shown that L_b satisfies the hypotheses of this Lemma and has at most k vertices.

Since C_1 is a clique in G and $C_1 \subset V(L_b)$, C_1 is a clique in L_b . Thus the inductive hypothesis implies that either W is a clique or there exists a vertex $x \in W - C_1$ such that $D(x) = \emptyset$ in L_b . If W is a clique, we have $D(b) = \emptyset$ in L_b and $b \in W - C_1$ (because $b \in V(D_b)$). Hence whether W is a clique or not, there exists a vertex $x \in W - C_1$ with $D(x) = \emptyset$ in L_b .

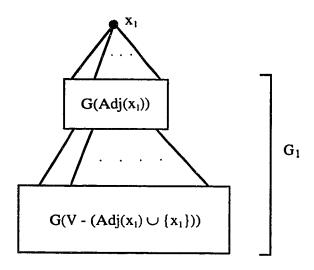
Since $x \in W - C_1$ and $W = C_1 \cup V(D_b)$, $x \in V(D_b)$. This means x is not adjacent to any vertex of $V - V(L_b)$ because such a vertex would be in a different component of $G(V - C_1)$. Thus $D(x) = \emptyset$ in G since $D(x) = \emptyset$ in L_b . Since $x \notin C_1$ and we assumed the vertices of $C - C_1$ were <u>not</u> in $V(D_b)$, we conclude that $x \notin C$.

4.4.16 Lemma. [Ros] Let G = (V, E) be a connected graph such that for each a, b ∈ V with a ∉ Adj(b), every minimal a, b separator of G is a clique. (4.4.17)

Then there exists an ordering σ of V such that for all $x \in V$, $MD(x) = \emptyset$ (in G_{σ}).

Proof. The proof is by induction on the number of vertices, |V|, and the case |V| = 1 is true vacuously. Suppose the Lemma is true for a graph which has k vertices. Let G = (V, E) be a graph with k+1 vertices satisfying the hypotheses of the Lemma. If G is complete, note that for any ordering σ of V and any $x \in V$, $MD(x) = \emptyset$ in G_{σ} . So suppose G is not complete.

By Lemma 4.4.14 and hypothesis (4.4.17), there exists a vertex x_1 with $D(x_1) = \emptyset$ in G. Let G_1 be the x_1 -elimination graph. It is connected by Lemma 4.4.6. We claim that G_1 satisfies hypothesis (4.4.17). Since $D(x_1) = \emptyset$ in G, $Adj(x_1)$ is a clique in G. Thus $Adj(x_1) \cup \{x_1\}$ is a clique in G which implies $V - (Adj(x_1) \cup \{x_1\}) \neq \emptyset$ since V is not a clique. So $Adj(x_1)$ separates x_1 from each vertex in $V - (Adj(x_1) \cup \{x_1\})$. Hence $Adj(x_1)$ is a separation clique in G (see picture).



Since $D(x_1) = \emptyset$ in G, $G_1 = (V - \{x_1\}, E(V - \{x_1\}))$. So the leaves of G with respect to $Adj(x_1)$ are $G(Adj(x_1) \cup \{x_1\})$ and G_1 . Thus, if a and b are vertices in G_1 with a $\notin Adj(b)$ in G_1 , then any minimal a, b separator of G_1 is also a minimal a, b separator of G by Lemma 4.4.13(ii), hence is a clique by (4.4.17). Thus G_1 satisfies hypothesis (4.4.17) and has k vertices. So by the inductive hypothesis, there exists an ordering τ of the vertices of G_1 such that for all $x \in V - \{x_1\}$, $MD(x) = \emptyset$ (in $(G_1)_{\tau}$). Let $\tau(i) = x_{i+1}$ for i = 1, ..., k.

Now in G choose the ordering $\sigma(i) = \tau(i-1) = x_i$ for i=2,...,k+1 and $\sigma(1) = x_1$. Since $D(x_1) = \emptyset$ in G, $MD(x_1) = \emptyset$ in G_{σ} . Furthermore, since σ preserves the order of the vertices established by τ , and $G_1 = G(V - \{x_1\})$, and for each $x \in V - \{x_1\}$, $MD(x) = \emptyset$ in $(G_1)_{\tau}$, it follows that $MD(x_i) = \emptyset$ in G_{σ} for i = 2, ..., k + 1. Thus we have found an ordering σ of the vertices of G such that for all $x \in V$, $MD(x) = \emptyset$ in G_{σ} .

Proof of Theorem 4.4.10. (1) \Rightarrow (2) by Lemma 4.4.11; (2) \Rightarrow (3) by Lemma 4.4.12; and (3) \Rightarrow (1) by Lemma 4.4.16 and Lemma 4.4.9.

4.4.18 Corollary. A graph G has a perfect elimination ordering if and only if G is chordal.

Proof. If G is connected, this corollary follows at once from Theorem 4.4.10 and Lemma 4.4.9.

Otherwise, G has two or more components. If G is chordal, then each component is chordal which implies each component has a perfect elimination ordering from above. If we sequentially list the vertices of each component according to its perfect elimination ordering, then any concatenation of these lists defines a perfect elimination ordering of the vertices of G.

Conversely, suppose G has a perfect elimination ordering σ . Then G_{σ} is monotone transitive. Since monotone transitivity is passed on from ordered graphs to subgraphs inheriting the same ordering, if we sequentially list the vertices in each component according to their order in σ , this defines a perfect elimination ordering for each component by Lemma 4.4.9. Thus by the first part of this proof, each component is chordal which implies G is chordal since any cycle must be contained within a single component.

4.5 Completable Graphs and Chordality

In this section, we will prove the following major result.

4.5.1 Theorem. [GJSW] Let G be a graph which contains all possible loops. Then G is completable if and only if G is chordal.

From section 4.4, we know chordal graphs are exactly those graphs which have perfect elimination orderings. Here we show that given any chordal graph G, it is possible to add one edge at a time to get a sequence of chordal graphs culminating with the complete graph. The following four lemmas provide the foundation for this result. As discussed toward the beginning of section 4.4, we will use the sequence of chordal graphs to establish an order for specifying entries in a G-partial positive definite matrix, and will show that numbers can always be found to substitute into the unspecified positions so that the completion is positive definite.

4.5.2 Lemma. [LRT] Let σ be a perfect elimination ordering of a chordal graph G = (V, E), and let $x \in V$. Then σ is also a perfect elimination ordering of $G' = (V, E \cup D(x))$.

Proof. Consider the ordering σ on G'. To see that this is a perfect elimination ordering of G', we will show G'_{σ} is monotone transitive. Let $y \in V$ and suppose $w, z \in MAdj(y)$ in G'_{σ} with $w \neq z$. We will now show that $\{w, z\} \in E \cup D(x)$.

There are three cases. (Case 1) Suppose $\{w,y\}$, $\{z,y\} \in E$. Then $w,z \in MAdj(y)$ in G_{σ} , and since σ is perfect in G, G_{σ} is monotone transitive. Thus $w \in Adj(z)$ in G, i.e., $\{w,z\} \in E$.

(Case 2) Suppose $\{w, y\}$, $\{z, y\} \in D(x)$. Then $w, z \in Adj(x)$ in G which implies $\{w, z\} \in E$ or $\{w, z\} \in D(x)$.

(Case 3) Suppose without loss of generality that $\{w, y\} \in E$ and $\{z, y\} \in D(x)$. Then $z, y \in Adj(x)$ in G and $\{z, y\} \notin E$. If w = x, then $\{w, z\} = \{x, z\} \in E$ since $z \in Adj(x)$ in G. So suppose $w \neq x$. We will show $\{w, x\} \in E$ which, together with the fact that $\{z, x\} \in E$, imply $\{w, z\} \in E \cup D(x)$.

We claim first that $x \in MAdj(y)$ in G_{σ} . Since $\{x, y\} \in E$ by assumption, we need only show $\sigma^{-1}(x) > \sigma^{-1}(y)$. Suppose on the contrary that $\sigma^{-1}(x) < \sigma^{-1}(y)$. Since $z \in MAdj(y)$ in G'_{σ} by hypothesis, $\sigma^{-1}(z) > \sigma^{-1}(y)$. So $\sigma^{-1}(z) > \sigma^{-1}(x)$. Since we know $z \in Adj(x)$ in G, it follows that $z \in MAdj(x)$ in G_{σ} . So we have $y, z \in MAdj(x)$ in G_{σ} , and $y \neq z$ by their definitions. Since σ is perfect in G, G_{σ} is monotone transitive. So $y \in Adj(z)$ in G, i.e., $\{z, y\} \in E$ which contradicts the fact that $\{z, y\} \notin E$. Therefore, we conclude that $\sigma^{-1}(x) > \sigma^{-1}(y)$ and $x \in MAdj(y)$ in G_{σ} .

Now we have $x \in MAdj(y)$ in G_{σ} , and by assumption, $w \in MAdj(y)$ in G'_{σ} (and hence in G_{σ} because $\{w, y\} \in E$) and $w \neq x$. Thus since σ is perfect in G, G_{σ} is monotone transitive; so $w \in Adj(x)$ in G, i.e., $\{w, x\} \in E$. Finally, since we also know $\{z, x\} \in E$, we must have $\{w, z\} \in E$ or $\{w, z\} \in D(x)$.

4.5.3 <u>Lemma</u>. [LRT] If G = (V, E) is chordal and $x \in V$, then the elimination graph G_x is chordal.

Proof. Let G = (V, E) be chordal and let $x \in V$. Then by Corollary 4.4.18 and Lemma 4.5.2, $G' = (V, E \cup D(x))$ is chordal. The elimination graph G_x is equal to $(V - \{x\}, E(V - \{x\}) \cup D(x))$ which is obtained from G' by eliminating x and its incident edges. Suppose G_x is not chordal. Then it contains a nonchorded cycle μ of length ≥ 4 . Since $x \notin \mu$, and the edges of G' are just those of G_x together with any edges incident to x

(in G), μ has no chord in G'. This contradicts the fact that G' is chordal. Hence we conclude that G_x is chordal.

4.5.4 Lemma. [LRT] Let G = (V, E) be a chordal graph, and let x be any vertex such that $D(x) = \emptyset$. Then G has a perfect elimination ordering σ with $\sigma(1) = x$. Proof. Let |V| = n. By Corollary 4.4.18, there exists a perfect elimination ordering τ of V, say $\tau(k) = x$ for some $k \in \{1, ..., n\}$ and $\tau(i) = x_i$ for $i \neq k$. If k = 1, we are done. Otherwise, by Lemma 4.4.9, G_{τ} is monotone transitive; so for each $v \in V$, if $w, y \in MAdj(v)$ in G_{τ} , then $w \in Adj(y)$ or w = y.

Now define a new ordering σ by $\sigma(1) = x$, $\sigma(i) = x_{i-1}$ for $2 \le i \le k$, and $\sigma(i) = x_i$ for i > k. For each $v \in V - \{x\}$, if $w, y \in MAdj(v)$ in G_{σ} , then $w, y \in MAdj(v)$ in G_{τ} ; hence we still have $w \in Adj(y)$ or w = y. If $w, y \in MAdj(x)$ in G_{σ} , then $w, y \in Adj(x)$; and since $D(x) = \emptyset$, we must have $w \in Adj(y)$ or w = y. Hence G_{σ} is monotone transitive; so σ is another perfect elimination ordering of V.

4.5.5 <u>Lemma.</u> [LRT] Let G = (V, E) be a chordal graph. Suppose F is another set of edges such that $F \neq \emptyset$, $E \cap F = \emptyset$, and $G' = (V, E \cup F)$ is also chordal. Then there exists some $f \in F$ such that $G' - f = (V, E \cup F - \{f\})$ is chordal.

Proof. The proof is by induction on n = |V|, the number of vertices. If $n \le 3$, the result is immediate since any graph with three or fewer vertices is chordal. Suppose the Lemma is true for chordal graphs satisfying the hypotheses of the Lemma with n_0 or fewer vertices.

Let G and G' be chordal graphs satisfying the hypotheses of the Lemma with $n = n_0 + 1$.

Let $R = \{x \in V: D(x) = \emptyset\}$, where D(x) is the deficiency in G. Let

 $S = \{x \in V: D'(x) = \emptyset\}$, where D'(x) is the deficiency in G'. Since G is chordal, there is a perfect elimination ordering φ of the vertices of G; suppose $\varphi(i) = x_i$ for i = 1, ..., n. Then by Lemma 4.4.9, $D(x_1) = \emptyset$ in G. Hence $R \neq \emptyset$. A similar argument shows that $S \neq \emptyset$. There are now two cases to consider.

(Case 1) Suppose for some $x \in S$, there exists an edge $f = \{u, x\} \in F$. Since $D'(x) = \emptyset$, G' has a perfect elimination ordering τ with $\tau(1) = x$ by Lemma 4.5.4. Therefore G'_{τ} is monotone transitive and $x \notin MAdj(y)$ in G'_{τ} for any y. So deleting f from G' preserves monotone transitivity relative to τ ; hence τ is also a perfect elimination ordering for G' - f. Thus by Corollary 4.4.18, G' - f is chordal.

(Case 2) Suppose Case 1 does not hold. Then both endpoints of any edge in F must have nonempty deficiencies in G'.

We first prove that there exists an $x \in S$ such that $F \nsubseteq D(x)$, i.e., there is an edge in F that is not in D(x). Pick any $z \in S$. Because $D'(z) = \emptyset$, $D(z) \subseteq F$. If $F \nsubseteq D(z)$, let x = z. Otherwise, since $D(z) \subseteq F$, F = D(z). In this case, let x be any vertex in R, i.e., with $D(x) = \emptyset$. By Lemma 4.5.4, G has a perfect elimination ordering G with G(x) = 0. In addition, since G(x) = 0, G(x) = 0 by Lemma 4.5.2. Since G(x) = 0 by Lemma 4.4.9, i.e., G(x) = 0 by Lemma 4.5.2.

Let $x \in S$ with $F \nsubseteq D(x)$. Let F' be the set of edges in F that are not in D(x); so $F = D(x) \cup F'$. Note that $G_x = (V - \{x\}, E(V - \{x\}) \cup D(x))$ and $G'_x = (V - \{x\}, (E \cup F)(V - \{x\}) \cup D'(x))$ are chordal by Lemma 4.5.3. We claim G'_x is obtained by adding the set of edges F' to G_x . Since $x \in S$, $D'(x) = \emptyset$; furthermore, since we are in Case 2, no edge incident to x can be in F. Thus the set of edges of G'_x is

 $(E \cup F)(V - \{x\}) = E(V - \{x\}) \cup F = E(V - \{x\}) \cup D(x) \cup F'$. Hence G_x and G_x' satisfy the hypotheses of this Lemma and each has n_0 vertices. So by the inductive hypothesis, there exists an $f \in F' = F - D(x)$ such that $G_x' - f$ is chordal.

We claim that G' - f is chordal. For otherwise G' - f would contain a nonchorded cycle μ of length $\ell \ge 4$. Since G' is chordal, removing f causes this cycle to be nonchorded, which means ℓ must be 4. (Otherwise G' would contain a nonchorded cycle of length at least 4.) Suppose x is in the cycle, i.e., $\mu = [x, y_2, y_3, y_4, x]$. Since we are in Case 2, f is not incident to x; so $f = \{y_2, y_4\}$. Since $E \cap F = \emptyset$, $f \notin E$; so $f \in D(x)$ which contradicts the fact that $f \in F - D(x)$. Hence x is not in μ . So removing x and its incident edges from G' - f does not affect μ . But removing x and its incident edges from G' - f which means G'_x - f contains μ , i.e., G'_x - f is not chordal, a contradiction. Thus we conclude that G' - f is chordal.

4.5.6 Corollary. [GJSW] Let G = (V, E) be a chordal graph which is not the complete graph, and let s be the difference between the number of edges in the complete graph on IVI vertices and the number of edges in G. Then there exists a sequence of chordal graphs $G^{(i)}$, i = 0, 1,..., s, such that $G^{(0)} = G$, $G^{(s)}$ is the complete graph, and $G^{(i)}$ is obtained by adding an edge to $G^{(i-1)}$ for each i = 1,..., s.

Proof. Let $G^{(0)} = G$ and let $G^{(s)}$ be the complete graph on IVI vertices. Then $G^{(0)}$ and $G^{(s)}$ satisfy the hypotheses of Lemma 4.5.5; hence there exists an edge f_s in $G^{(s)}$ and not in $G^{(0)}$ such that $G^{(s-1)} \equiv G^{(s)} - f_s$ is chordal. Now $G^{(s-1)}$ and $G^{(0)}$ satisfy the hypotheses of Lemma 4.5.5 and we may continue the process, eventually obtaining the desired sequence of chordal graphs.

4.5.7 Lemma. [GJSW] Let G = (V, E) be a graph containing all possible loops. If $\{u, v\} \notin E$, let $G + \{u, v\}$ denote the graph G with the edge $\{u, v\}$ added. Then each cycle of length 4 in G has a chord if and only if the following holds.

For any pair of distinct vertices u and v with $\{u, v\} \notin E$, the union of all cliques in $G + \{u, v\}$ which contain both u and v is a clique in $G + \{u, v\}$.

Proof. (\Rightarrow) Suppose each cycle of length 4 in G has a chord. Let u and v be distinct vertices with $\{u, v\} \notin E$. Then the set whose elements are u and v is a clique in $G + \{u, v\}$ containing u and v. If this is the only such clique, we are done. Otherwise let C and C' be cliques in $G + \{u, v\}$ each of which contains u and v. We will show that $C \cup C'$ is a clique in $G + \{u, v\}$. It then follows that the union of all cliques in $G + \{u, v\}$ each of which contains u and v is a clique in $G + \{u, v\}$.

Let $z \in C$ and $z' \in C'$. We will show that $\{z, z'\}$ is an edge in $G + \{u, v\}$. There are three cases. (Case 1) Suppose z = z'. Then $\{z, z'\}$ is a loop, hence an edge in G, hence an edge in $G + \{u, v\}$. (Case 2) Suppose z equals u or v. Then z and z' are both in C' which implies $\{z, z'\}$ is an edge in $G + \{u, v\}$ since C' is a clique in $G + \{u, v\}$. Similarly, if z' equals u or v, then z and z' are both in C which implies $\{z, z'\}$ is an edge in $G + \{u, v\}$ since C is a clique in $G + \{u, v\}$. (Case 3) Suppose u, z, v, and z' are four distinct vertices. Then [u, z, v, z', u] is a cycle in G of length A, and it must have a chord. Thus either $\{u, v\}$ or $\{z, z'\}$ must be an edge in G. Since $\{u, v\} \notin E$ by assumption, $\{z, z'\} \in E$; hence $\{z, z'\}$ is an edge in $G + \{u, v\}$. Since C and C' are both cliques in $G + \{u, v\}$, and z and z' were chosen arbitrarily, we have shown that $C \cup C'$ is a clique in $G + \{u, v\}$.

(⇐) Conversely, suppose there exists a nonchorded cycle μ in G of length 4, say $\mu = [x, u, y, v, x]$. Then $\{x, y\}$, $\{u, v\} \notin E$. So $C = \{x, u, v\}$ and $C' = \{y, u, v\}$ are cliques in $G + \{u, v\}$ which contain u and v, but $C \cup C'$ is not a clique in $G + \{u, v\}$ since

 $\{x, y\} \notin E$. Thus the union of all cliques in $G + \{u, v\}$ which contain u and v is not a clique in $G + \{u, v\}$.

4.5.8 Remark. [GJSW] Observe that Lemma 4.5.7 can be restated as follows:
When G = (V, E) has all possible loops, each cycle of length 4 in G has a chord if and only if for any pair of distinct vertices u and v with {u, v} ∉ E, there is a unique maximal clique in G + {u, v} which contains both u and v.

The previous result is important because cliques in a graph G correspond to completely specified principal submatrices in any G-partial matrix. Suppose G is chordal, and we complete some G-partial positive definite matrix using a sequence of chordal graphs shown to exist in Corollary 4.5.6. Then 4.5.8 tells us that at each step, we will complete a unique largest principal submatrix. We will show that at each step, this largest principal submatrix can be made positive definite, which is enough to guarantee a positive definite completion of the original G-partial positive definite matrix.

So far in this section, we have concentrated on preparing to prove that chordality implies completability in 4.5.1. The following lemma will be used in proving the converse, i.e., if G is completable, then G is chordal.

4.5.9 Lemma. [GJSW] For each $k \in \mathbb{N}$, there is a unique k-by-k positive semidefinite matrix A which has 1's down the main, sub-, and superdiagonals. This matrix A is the matrix of all 1's.

Proof. Let $k \in \mathbb{N}$ and let A be the k-by-k matrix of all 1's. If k = 1, we are done. If $k \ge 2$, then A is positive semidefinite since A is Hermitian and the eigenvalues of A are

0 and k. (To see that k is an eigenvalue of A, consider the k-by-1 vector of all 1's. Also note that the rank of A is 1 which implies that the nullity of A is k - 1.)

Thus we need only show that A is the only $k \times k$ positive semidefinite matrix with 1's down the main, sub-, and superdiagonals. If k = 2, the result is immediate. For k = 3, let

$$A_0 = \begin{bmatrix} 1 & 1 & x \\ 1 & 1 & 1 \\ \overline{x} & 1 & 1 \end{bmatrix}$$
 be positive semidefinite, where $x \in \mathbb{C}$. Then

$$0 \le \det(A_0) = -(1 - \overline{x}) + x(1 - \overline{x}) = (-1 + x)(1 - \overline{x})$$
$$= -(1 - x)(1 - \overline{x}) = -(1 - x)(\overline{1 - x}) = -|1 - x|^2.$$

Thus $|1-x|^2 = 0$; hence x = 1. Thus we have shown that the matrix of all 1's is the only 3×3 positive semidefinite matrix with 1's down the main, sub-, and superdiagonals.

Now let $k \ge 4$ and let A_0 be $k \times k$ positive semidefinite with 1's down the main, sub-, and superdiagonals. Since A_0 is positive semidefinite, each 3×3 principal submatrix $A_0(i, i+1, i+2)$, i = 1, 2, ..., k-2, must also be positive semidefinite. In addition, since $A_0(i, i+1, i+2)$ has 1's down its main, sub-, and superdiagonals, it must be the 3×3 matrix of all 1's. Hence $[A_0]_{ij} = 1$ for |i - j| = 2, i.e., the second superdiagonal in A_0 and the second sub-diagonal in A_0 must be all 1's.

It now follows that each $A_0(i, i+1, i+3)$ is a 3×3 principal submatrix of A_0 with 1's down its main, sub-, and superdiagonals. Hence the same argument as above shows that its (1, 3)- and (3, 1)-entries must also be 1 which implies $[A_0]_{ij} = 1$ for |i - j| = 3. Continuing step-by-step in order for p = i+4,...,k, the same argument can be applied to each 3×3 principal submatrix $A_0(i, i+1, p)$ to show that $[A_0]_{ij} = 1$ for all i and j. Thus A_0 is the matrix of all 1's which completes the proof.

We are now ready to prove the main result of this chapter.

4.5.1 Theorem. [GJSW] Let G be a graph which contains all possible loops. Then G is completable if and only if G is chordal.

Proof. (\Rightarrow) Suppose G is completable. To obtain a contradiction, assume that G is not chordal. Then G contains a nonchorded cycle μ of length $k \ge 4$. Let G' be the graph on the vertices of μ induced by G. Then G' contains all possible loops. We may assume that the vertices of G' are numbered 1 through k, in the same order that they appear in μ . (If the vertices start out numbered differently, a suitable permutation similarity of any G-partial Hermitian matrix A(G) is equivalent to renumbering the vertices of G according to the desired order. This yields a new G-partial Hermitian matrix A'(G) whose leading $k \times k$ principal submatrix is G'-partial Hermitian. And since similar matrices have the same eigenvalues, A(G) will have a positive definite completion if and only if A'(G) has a positive definite completion.)

Now, in any G'-partial matrix, the only specified positions are the (1, k) and (k, 1) positions and those on the main, sub-, and superdiagonals. Let $\epsilon > 0$ and define a G'-partial Hermitian matrix A(G') as follows:

$$[A(G')]_{ii} = 1 + \epsilon \text{ for } i = 1,..., k;$$

$$[A(G')]_{i,i+1} = [A(G')]_{i+1,i} = 1 \text{ for } i = 1,..., k-1;$$
 and
$$[A(G')]_{1k} = [A(G')]_{k1} = -1.$$

Then A(G') is G'-partial positive definite since its only completely specified principal submatrices are $\begin{bmatrix} 1+\epsilon & 1 \\ 1 & 1+\epsilon \end{bmatrix}$ and $\begin{bmatrix} 1+\epsilon & -1 \\ -1 & 1+\epsilon \end{bmatrix}$, both of which are positive definite.

Extend A(G') to a G-partial Hermitian matrix $A_{\epsilon}(G)$ as follows. Let A(G') be the leading $k \times k$ principal submatrix of $A_{\epsilon}(G)$; let $[A_{\epsilon}(G)]_{ii} = 1 + \epsilon$ for i > k; and let $[A_{\epsilon}(G)]_{ij} = 0$ whenever $\{x_i, x_j\}$ is an edge in G but not in G', where x_i and x_j are the vertices numbered i and j, respectively. We claim that $A_{\epsilon}(G)$ is G-partial positive definite. Any completely specified principal submatrix of $A_{\epsilon}(G)$ has one of three forms: (1) It is

a principal submatrix of A(G'), hence positive definite since A(G') is G'-partial positive definite. (2) It is a principal submatrix of $(1 + \varepsilon)I$, hence positive definite. (3) It has the form $\begin{bmatrix} B & 0 \\ 0 & (1+\epsilon)I \end{bmatrix}$, where B is a principal submatrix of A(G'). Since A(G') is G'-partial positive definite, B is positive definite. Let $\begin{bmatrix} x \\ y \end{bmatrix}$ be any appropriately blocked, nonzero

complex vector of appropriate size. Then
$$\begin{bmatrix} x^* & y^* \end{bmatrix} \begin{bmatrix} B & 0 \\ 0 & (1+\epsilon)I \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = x^*Bx + y^*(1+\epsilon)Iy$$

which must be positive because both summands are nonnegative, and at least one is positive since $\begin{vmatrix} x \\ y \end{vmatrix} \neq \theta$. Thus we have shown that each completely specified principal submatrix of $A_{\varepsilon}(G)$ is positive definite, i.e., $A_{\varepsilon}(G)$ is G-partial positive definite.

Since G is completable, there exists a positive definite completion B_{ε} of $A_{\varepsilon}(G)$ for each $\epsilon > 0$. Consider the sequence $\left\langle B_{1/i} \right\rangle_{i=1}^{\infty}$ in S, the set of all positive semidefinite $n \times n$ matrices, where $B_{1/i}$ is a positive definite completion of $A_{1/i}(G)$ for each $i \in \mathbb{N}$. Since each diagonal entry of each matrix in the sequence is specified and lies in the interval (1, 2], the sequence is bounded by Lemma 3.1.2. Thus it has a convergent subsequence whose limit, B_0 , is such that $B_0(k)$ has 1's down its main, sub-, and superdiagonals and -1 in its (1, k) and (k, 1) positions. Since S is closed (in H) by Theorem 1.1.11, B₀ must be positive semidefinite which implies B₀(k) is positive semidefinite. But no such positive semidefinite matrix exists by Lemma 4.5.9. Thus we have a contradiction, and we conclude that any cycle of length ≥ 4 in G has a chord, i.e., G is chordal.

 (\Leftarrow) Suppose G = (V, E) is a chordal graph. If G is the complete graph, we are done since any G-partial positive definite matrix has all entries specified, and is therefore positive definite. So assume G is not the complete graph, and let s be the difference between the number of edges in the complete graph on |V| vertices and the number of edges in G. By Corollary 4.5.6, there exists a sequence of chordal graphs, $G = G^{(0)}, G^{(1)}, \dots, G^{(s)}$, where

 $G^{(s)}$ is the complete graph on IVI vertices, and $G^{(i)}$ is obtained by adding an edge to $G^{(i-1)}$ for each i = 1, ..., s.

Let $A = [a_{kp}]$ be any G-partial positive definite matrix. We must show that A has a positive definite completion. We will show that there exists a $G^{(1)}$ -partial positive definite matrix $A_1 = \left[a_{kp}^{(1)}\right]$ such that $a_{kp}^{(1)} = a_{kp}$ for each $\{x_k, x_p\} \in E$, where x_k and x_p are the vertices numbered k and p, respectively. (So A_1 will be the same as A, except A_1 will have two more entries specified—those corresponding to the added edge in $G^{(1)}$.) Once we know such A_1 can be found, the same argument can be used to show that if $i \in \{1, ..., s-1\}$ and A_i is a $G^{(i)}$ -partial positive definite matrix, then there exists a $G^{(i+1)}$ -partial positive definite matrix A_{i+1} such that $a_{kp}^{(i+1)} = a_{kp}^{(i)}$ for each edge $\{x_k, x_p\}$ in $G^{(i)}$. Since a $G^{(s)}$ -partial positive definite matrix A_s has all entries specified, it follows that A_s will be a positive definite completion of A. So we just need to establish the existence of a matrix A_1 as defined above.

Let $\{u, w\}$ be the edge of $G^{(1)}$ that is not in G. Then by 4.5.8, there is a unique maximal clique C in $G^{(1)}$ which contains both u and w. By the permutation similarity argument given in the (\Rightarrow) part of this proof, we may assume without loss of generality that the vertices of G have been numbered so that $C = \{x_1, ..., x_q\}$, $u = x_1$ and $w = x_q$. The only edge missing in G(C), the graph on C induced by G, is $\{x_1, x_q\}$ since C is a clique in $G^{(1)} = G + \{x_1, x_q\}$. Hence for $1 \le i, j \le q$, $\{x_i, x_j\}$ is an edge in G(C) if and only if $|i-j| \le q-2$. Thus G(C) is a band graph which implies it is completable by Corollary 4.3.3. Any completely specified principal submatrix of A(1, ..., q) is also a completely specified principal submatrix of A, hence is positive definite. So A(1, ..., q) is G(C)-partial positive definite, thus has a positive definite completion because G(C) is completable. Let $A_1(1, ..., q)$ be a positive definite completion of A(1, ..., q).

Let A_1 be the $G^{(1)}$ -partial matrix whose leading $q \times q$ principal submatrix is

 $A_1(1,...,q)$, and whose (k,p)-entry equals a_{kp} for each $\{x_k,x_p\}\in E$. We claim that A_1 is $G^{(1)}$ -partial positive definite. Any completely specified principal submatrix of A is positive definite. Thus, since A and A_1 differ only in the (1,q) and (q,1) positions, we need only check that any completely specified principal submatrix of A_1 which includes rows 1 and q is positive definite. Since C is the maximal clique in $G^{(1)}$ containing x_1 and x_q , and cliques correspond to completely specified principal submatrices, any completely specified principal submatrix of A_1 which includes rows 1 and q is a principal submatrix of $A_1(1,...,q)$, hence must be positive definite because $A_1(1,...,q)$ is positive definite. Thus we have shown that A_1 is $G^{(1)}$ -partial positive definite which completes the proof.

4.6 An Algorithm for Constructing a Perfect Elimination Ordering

4.6.1 Let G = (V, E) be a chordal graph. We begin with all vertices unnumbered. The following algorithm from [LRT] will number the vertices from n to 1. The algorithm also assigns to each vertex v a sequence s(v) which is a subset of $\{1, ..., n\}$, listed in decreasing order. We will order the set of sequences lexicographically, i.e., given two sequences $s(v) = [p_1, p_2, ..., p_k]$ and $s(w) = [q_1, q_2, ..., q_r]$, we define s(v) < s(w) if, for some l, $p_i = q_i$ for i = 1, 2, ..., l, and either $p_{l+1} < q_{l+1}$, or k = l and k < r. If k = r and $p_i = q_i$, $1 \le i \le k$, then s(v) = s(w).

4.6.2 ALGORITHM LEX P: begin

assign the initial sequence Ø to all vertices;

for i = n step -1 until 1 do begin

select: pick any unnumbered vertex v with maximal sequence;

comment: assign v the number i, $\sigma(i) = v$;

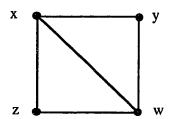
update: for each unnumbered vertex $w \in Adj(v)$ do

adjoin i to the sequence of w;

end end LEX P.

4.6.3 Notation. It will be helpful to let $s_k(v)$ denote the sequence assigned to v by LEX P just before the number k is assigned to a vertex. Note that $s_n(v) = \emptyset$ for all v.

4.6.4 Example. Consider the graph



Two examples of perfect elimination orderings and the associated sequences are given below. Both orderings are generated by running through LEX P. Differences arise when two or more unnumbered vertices have the same (maximal) sequence at a given step. Numbering a different vertex at this step yields a different perfect elimination ordering. Note that it is not the final sequences but the sequences at each step which are important in determining the ordering.

$$s_4(x) = \emptyset = s_4(y) = s_4(z) = s_4(w);$$
 $\sigma_1(4) = x$

$$s_3(y) = [4] = s_3(z) = s_3(w);$$
 $\sigma_1(3) = y$

$$s_2(w) = [4, 3], s_2(z) = [4];$$
 $\sigma_1(2) = w$

$$s_1(z) = [4, 2];$$
 $\sigma_1(1) = z$

$$s_4(x) = \emptyset = s_4(y) = s_4(z) = s_4(w);$$
 $\sigma_2(4) = z$

$$s_3(x) = [4] = s_3(w), s_3(y) = \emptyset;$$
 $\sigma_2(3) = x$

$$s_2(w) = [4, 3], s_2(y) = [3];$$
 $\sigma_2(2) = w$

$$s_1(y) = [3, 2];$$
 $\sigma_2(1) = y$

4.6.5 Theorem. Given a chordal graph G = (V, E), the algorithm LEX P yields a perfect elimination ordering of V.

Proof. Apply LEX P to G and let σ be the resulting ordering of V. For each $v \in V$, we will show MAdj(v) is a clique which implies MD(v) = \emptyset , hence σ is a perfect elimination ordering of V. Let x_k be the vertex assigned the number k by LEX P (or equivalently, by σ). Observe that after LEX P has run its course, the following is true [LRT].

For each $v \in V$, $k \in s(v)$ if and only if $x_k \in MAdj(v)$. (4.6.6) Suppose, trying for a contradiction, that $MAdj(x_{j_0})$ is not a clique for some $x_{j_0} \in V$. Then there exist two vertices $x_{j_1}, x_{j_2} \in MAdj(x_{j_0})$ such that $\{x_{j_1}, x_{j_2}\} \notin E$. Assume without loss of generality that $j_2 > j_1$. Then $j_2 > j_1 > j_0$, and by (4.6.6), we also have $j_2 \in s(x_{j_0})$ and $j_2 \notin s(x_{j_1})$.

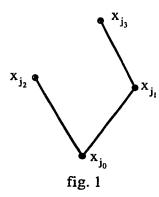
Observe that the following is true.

For any $v \in V$, $x_m \in MAdj(v)$ if and only if for each k < m, $m \in s_k(v)$. (4.6.7) Note that if $x_m \notin MAdj(v)$, then there exists k < m such that $m \notin s_k(v)$ which implies $m \notin s_i(v)$ for each i < m.

(Case 1) Suppose
$$s_{j_2}(x_{j_0}) \ge s_{j_2}(x_{j_1})$$
. Because x_{j_0} is adjacent to x_{j_2} ,
$$s_{j_2-1}(x_{j_0}) = [s_{j_2}(x_{j_0}), j_2]$$
$$> s_{j_2}(x_{j_0})$$
$$\ge s_{j_2}(x_{j_1})$$
$$= s_{j_2-1}(x_{j_1}).$$

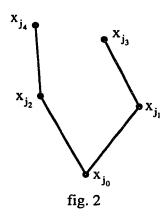
Once the sequence of one vertex is greater than the sequence of another as LEX P runs its course, it will be greater thereafter, i.e., if v and w are in V and $s_k(v) > s_k(w)$ for any k, then $s_p(v) > s_p(w)$ for all p < k. Thus $s_{j_1}(x_{j_0}) > s_{j_1}(x_{j_1})$ which implies x_{j_1} would not receive the number j_1 , a contradiction. So Case 1 cannot happen because of the way LEX P assigns labels and numbers.

(Case 2) Suppose $s_{j_2}(x_{j_1}) > s_{j_2}(x_{j_0})$. We will see that this case is impossible because G is chordal and finite. For some nonnegative integer l, the first l elements of $s_{j_2}(x_{j_1})$ and $s_{j_2}(x_{j_0})$ agree, and either the (l+1)st element of $s_{j_2}(x_{j_1})$ is greater than the (l+1)st element of $s_{j_2}(x_{j_0})$, or $s_{j_2}(x_{j_1})$ has an (l+1)st element but $s_{j_2}(x_{j_0})$ has only l elements. In either case, the (l+1)st element of $s_{j_2}(x_{j_1})$ belongs to $s_{j_2}(x_{j_1})$ but not to $s_{j_2}(x_{j_0})$. That is, there exists $j_3 > j_2$ such that $j_3 \in s_{j_2}(x_{j_1})$ but $j_3 \notin s_{j_2}(x_{j_0})$. Thus $j_3 \in s(x_{j_1})$ but $j_3 \notin s(x_{j_0})$, hence $\{x_{j_1}, x_{j_3}\} \in E$, but $\{x_{j_0}, x_{j_3}\} \notin E$ by (4.6.6). We may assume without loss of generality that j_3 is the largest number that appears in $s(x_{j_1})$ but not in $s(x_{j_0})$, i.e., $s_k(x_{j_1}) = s_k(x_{j_0})$ for $k \ge j_3$. Because $\{x_{j_1}, x_{j_2}\}$, $\{x_{j_0}, x_{j_3}\} \notin E$, we cannot have $\{x_{j_2}, x_{j_3}\} \in E$ because that would yield a nonchorded cycle of length 4 in G (see fig. 1; loops have been left out for easier viewing).



Because $j_2 > j_1$, we must have $s_{j_2}(x_{j_2}) \ge s_{j_2}(x_{j_1})$. Since $x_{j_3} \in MAdj(x_{j_1})$ but $x_{j_3} \notin MAdj(x_{j_2})$, it follows that $j_3 \in s_{j_2}(x_{j_1})$ but $j_3 \notin s_{j_2}(x_{j_2})$ by (4.6.7). Thus $s_{j_2}(x_{j_2}) \ne s_{j_2}(x_{j_1})$ which implies $s_{j_2}(x_{j_2}) > s_{j_2}(x_{j_1})$. So as before, there is a largest j_4 in $s_{j_2}(x_{j_2})$ which is not in $s_{j_2}(x_{j_1})$. If $j_4 \le j_3$, j_3 must belong to both sequences, but it does not. So $j_4 > j_3$. Since $j_4 \in s(x_{j_2})$ but $j_4 \notin s(x_{j_1})$, $\{x_{j_2}, x_{j_4}\} \in E$, but $\{x_{j_1}, x_{j_4}\} \notin E$ by (4.6.6). From above, we have $s_k(x_{j_1}) = s_k(x_{j_0})$ for $k \ge j_3$, and $j_4 \notin s(x_{j_1})$. So we must

have $j_4 \notin s(x_{j_0})$ which implies $\{x_{j_0}, x_{j_4}\} \notin E$ by (4.6.6). Therefore we cannot have $\{x_{j_3}, x_{j_4}\} \in E$ since that would create a nonchorded cycle of length 5 in G (see fig. 2).



Now suppose m is a positive integer ≥ 4 and $\mu = [x_{j_m}, x_{j_{m-2}}, x_{j_{m-4}}, ..., x_{j_0}, ..., x_{j_{m-3}}, x_{j_{m-1}}]$ is a chain such that $j_i < j_{i+1}$ for each $i \in \{0, ..., m-1\}$, and any two nonconsecutive vertices in μ are not adjacent in G.

(§) Suppose further that for each $r \in \{0, ..., m-3\}$, j_{r+3} is the largest number that appears in $s(x_{j_{r+1}})$ but not in $s(x_{j_r})$, i.e., $s_k(x_{j_{r+1}}) = s_k(x_{j_r})$ for $k \ge j_{r+3}$.

Because $j_{m-1} > j_{m-2}$, we must have $s_{j_{m-1}}(x_{j_{m-1}}) \ge s_{j_{m-1}}(x_{j_{m-2}})$. Since $x_{j_m} \in MAdj(x_{j_{m-2}})$ but $x_{j_m} \notin MAdj(x_{j_{m-1}})$, it follows that $j_m \in s_{j_{m-1}}(x_{j_{m-2}})$ but $j_m \notin s_{j_{m-1}}(x_{j_{m-1}})$ by (4.6.7). Thus $s_{j_{m-1}}(x_{j_{m-1}}) \ne s_{j_{m-1}}(x_{j_{m-2}})$ which implies $s_{j_{m-1}}(x_{j_{m-1}}) > s_{j_{m-1}}(x_{j_{m-2}})$. So as before, there is a largest j_{m+1} in $s_{j_{m-1}}(x_{j_{m-1}})$ which is not in $s_{j_{m-1}}(x_{j_{m-2}})$. If $j_{m+1} \le j_m$, j_m must belong to both sequences, but it does not. So $j_{m+1} > j_m$. Since $j_{m+1} \in s(x_{j_{m-1}})$ but $j_{m+1} \notin s(x_{j_{m-2}})$, $\{x_{j_{m-1}}, x_{j_{m+1}}\} \in E$, but $\{x_{j_{m-2}}, x_{j_{m+1}}\} \notin E$ by (4.6.6).

Since $s_k(x_{j_{m-2}}) = s_k(x_{j_{m-3}})$ for $k \ge j_m$ by (§), and $j_{m+1} \notin s(x_{j_{m-2}})$ from above, we must have $j_{m+1} \notin s(x_{j_{m-3}})$ which implies $\{x_{j_{m-3}}, x_{j_{m+1}}\} \notin E$ by (4.6.6). Similarly, $s_k(x_{j_{m-3}}) = s_k(x_{j_{m-4}})$ for $k \ge j_{m-1}$ by (§), and $j_{m+1} \notin s(x_{j_{m-3}})$ from above; so $j_{m+1} \notin s(x_{j_{m-4}})$ which implies $\{x_{j_{m-4}}, x_{j_{m+1}}\} \notin E$ by (4.6.6). The same argument can be repeated to show

that $\{x_{j_{\ell}}, x_{j_{m+1}}\} \notin E$ for $\ell = 0, ..., m-3$. Therefore we cannot have $\{x_{j_m}, x_{j_{m+1}}\} \in E$ because that would create a nonchorded cycle of length > 4 in G.

Now we have a chain $[x_{j_{m+1}}, x_{j_{m-1}}, x_{j_{m-3}}, ..., x_{j_0}, ..., x_{j_{m-4}}, x_{j_{m-2}}, x_{j_m}]$ which is one link longer than μ and which shares the same characteristics, allowing the preceding argument to be applied again. Thus by the principle of induction, G must contain a chain of infinite length which contradicts the fact that G is finite. So in Case 2, we have also reached a contradiction. Hence we conclude that MAdj(v) is a clique for each v in V which completes the proof.

4.7 An Algorithm for Constructing a Sequence of Chordal Graphs

Let G = (V, E) be a chordal graph which contains all possible loops, and let A be a G-partial positive definite matrix. Let s be the difference between the number of edges in the complete graph on |V| = n vertices and the number of edges in G. Then A has 2s unspecified positions. The proof of Theorem 4.5.1 showed that A can be completed to a positive definite matrix by filling in its unspecified positions two at a time, using a sequence of chordal graphs, $G = G^{(0)}, G^{(1)}, \ldots, G^{(s)}$, shown to exist in Corollary 4.5.6. This results in a sequence of matrices, $A = A_0, A_1, \ldots, A_s$, where A_i is $G^{(i)}$ -partial positive definite, and A_s is the desired completion.

We will now show how to actually construct a sequence of chordal graphs which satisfies the conditions of Corollary 4.5.6. First use the algorithm from the previous section to obtain a perfect elimination ordering σ for G. For k = 1,..., n, let x_k be the vertex numbered $\sigma^{-1}(k)$. Using the notation from Corollary 4.5.6, define inductively the following sequence of graphs, $G^{(0)} = (V, E^{(0)}),..., G^{(s)} = (V, E^{(s)})$, where $E^{(i)}$ denotes the edges in $G^{(i)}$:

$$G^{(0)} = G, (4.7.1)$$

and for i = 0, ..., s - 1,

$$G^{(i+1)} = G^{(i)} + \{x_{k_i}, x_{r_i}\}, \qquad (4.7.2)$$

where $k_i = \max\{k: \{x_k, x_m\} \notin E^{(i)} \text{ for some } m\}$, and $r_i = \max\{r: \{x_r, x_{k_i}\} \notin E^{(i)}\}.$

Note that $r_i < k_i$, i = 0,..., s - 1, since if r_i were larger, it would have been chosen as k_i , and $r_i \ne k_i$ because we are assuming G contains all possible loops.

4.7.3 Theorem. [GJSW] If σ is a perfect elimination ordering for $G = G^{(0)}$, then σ is a perfect elimination ordering for each of the graphs $G^{(1)}, \ldots, G^{(s)}$ defined inductively by (4.7.1)-(4.7.2). (Hence $G^{(i)}$ is chordal for $i = 1, \ldots, s$ by Corollary 4.4.18.) Proof. Let $i \in \{1, \ldots, s\}$ and $k \in \{1, \ldots, n\}$. We will show that $MD(x_k) = \emptyset$ in $G^{(i)}_{\sigma}$, which implies σ is a perfect elimination ordering for $G^{(i)}$ by Lemma 4.4.9. If i = s, the result is immediate since $G^{(s)}$ is the complete graph, so the deficiency (and hence monotone deficiency) of each vertex is empty.

For $i \neq s$, we proceed by induction. Since σ is a perfect elimination ordering for $G^{(0)}$ by hypothesis, $MD(x_k) = \emptyset$ in $G^{(0)}_{\sigma}$ by Lemma 4.4.9. Let $j \in \{0, \ldots, s-2\}$ such that $MD(x_k) = \emptyset$ in $G^{(j)}_{\sigma}$. Then $MAdj(x_k)$ in $G^{(j)}_{\sigma}$ is a clique. If $x_k \neq x_{r_j}$, $MAdj(x_k)$ in $G^{(j)}_{\sigma}$ and $MAdj(x_k)$ in $G^{(j+1)}_{\sigma}$ are the same since $G^{(j+1)} = G^{(j)} + \{x_{k_j}, x_{r_j}\}$ and $k_j > r_j$. Thus $MAdj(x_k)$ in $G^{(j+1)}_{\sigma}$ is a clique which implies $MD(x_k) = \emptyset$ in $G^{(j+1)}_{\sigma}$. If $x_k = x_{r_j}$, then $MAdj(x_{r_j})$ in $G^{(j+1)}_{\sigma} = (MAdj(x_{r_j})$ in $G^{(j)}_{\sigma} \cup \{x_{k_j}\}$. Since $MAdj(x_{r_j})$ in $G^{(j)}_{\sigma}$ is a clique by the inductive hypothesis, we need only show that x_{k_j} is adjacent to each vertex in $MAdj(x_{r_j})$ in $G^{(j)}_{\sigma}$. But this follows at once from how k_j and r_j are defined. Hence $MAdj(x_{r_j})$ in $G^{(j+1)}_{\sigma}$ is a clique which implies $MD(x_{r_j}) = \emptyset$ in $G^{(j+1)}_{\sigma}$.

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