A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF ÇANKIRI KARATEKİN UNIVERSITY

POSITIVE DEFINITE COMPLETION PROBLEM IN GRAPH THEORY

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR
THE DEGREE OF MASTER OF SCIENCE
IN
MATHEMATICS

BY

ZAHRAA IHSAN ABDULWAHID ALSAUD

ÇANKIRI

2024

POSITIVE DEFINITE COMPLETION PROBLEM IN GRAPH THEORY

By Zahraa Ihsan Abdulwahid ALSAUD

May 2024

We certify that we have read this thesis and that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science

Advisor **:** Asst. Prof. Dr. Hanife VARLI

Examining Committee Members:

Chairman **:** Asst. Prof. Dr. Adalet ÇENGEL
Mathematics
Bartın University

Member **:** Asst. Prof. Dr. Hanife VARLI
Mathematics
Çankırı Karatekin University

Member **:** Asst. Prof. Dr. Celalettin KAYA
Mathematics
Çankırı Karatekin University

Approved for the Graduate School of Natural and Applied Sciences

Prof. Dr. Hamit ALYAR
Director of Graduate School

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Zahraa Ihsan Abdulwahid ALSAUD

ABSTRACT

POSITIVE DEFINITE COMPLETION PROBLEM IN GRAPH THEORY

Zahraa Ihsan Abdulwahid ALSAUD
Master of Science in Mathematics
Advisor: Asst. Prof. Dr. Hanife VARLI
May 2024

The main source used in the preparation of this thesis is the graduate textbook "Graphs and Matrices", Bapat (2014). Essentially, what we do is to study the twelfth chapter of the mentioned textbook to understand and explain the “positive definite completion problem in graph theory”, as can be understood from the title of the thesis. But of course, no part of the aforementioned book has been quoted exactly, a study has been put forward with our own words and our own sentences; almost every proof has been written in more detail, and parts of the book that were left to the reader have been explained completely and the subject has been presented more understandably. In addition to these, the sources listed in the references were also consulted. Especially, for the preparation of chapter one, we benefited greatly from Paziak and Odell (2007). To summarize: In the first chapter, preliminaries about matrix theory, which are needed to understand the thesis, are given. In the second and main chapter of the thesis, chordal graphs are defined, positive definite completion notion is given, and it is proved that a graph is positive definite completable if and only if it is chordal. In the third chapter, the last chapter before the conclusions and recommendation chapter, a brief literature review on the subject of the thesis is presented mainly by using the notes at the end of the twelfth chapter of the mentioned book.

2024, 47 pages

Keywords: Nonsingular completion, Chordal graphs, Positive definite completion

ÖZET

GRAF TEORİSİNDE POZİTİF TANIMLI TAMAMLAMA PROBLEMİ

Zahraa Ihsan Abdulwahid ALSAUD
Matematik, Yüksek Lisans
Tez Danışmanı: Dr. Öğr. Üyesi Hanife VARLI
Mayıs 2024

Bu tezin hazırlanmasında kullanılan başlıca kaynak, Bapat (2014)'in "Graphs and Matrices" başlıklı lisansüstü kitabıdır. Esas itibariyle bizim yaptığımız, tezin başlığından da anlaşılacağı üzere, "graf teorisinde pozitif tanımlı tamamlama problemi"ni anlamak ve anlatmak için, söz konusu kitabın on ikinci bölümünün çalışılmasından ibarettir. Fakat tabii ki mevzubahis kitabın herhangi bir kısmı aynen alıntılanmamış, kendi sözcüklerimiz ve kendi cümlelerimizle bir çalışma ortaya konulmuş ve hemen her ispat ayrıntılı bir şekilde yazılmış ve kitabın okuyucuya bırakılan bölümleri eksiksiz bir şekilde açıklanarak konu daha anlaşılır bir şekilde sunulmuştur. Bunlara ek olarak, referanslar kısmında listelenmiş olan kaynaklara da başvurulmuştur. Özellikle, birinci bölümün hazırlanmasında Paziak ve Odell (2007)'den çok fazla yararlandık. Özetlemek gerekirse: Birinci bölümde, tezin anlaşılması için gerekli olan matris teorisine ilişkin ön bilgiler verilmiştir. Tezin ikinci ve ana bölümünde ise, kordal graflar tanımlanmış, pozitif tanımlı tamamlama kavramı verilmiş ve bir grafın ancak ve ancak kordal olması durumunda pozitif tanımlı tamamlanabileceği ispatlanmıştır. Tezin üçüncü, sonuç ve öneriler bölümünden önceki son bölümünde ise, esas olarak adı geçen kitabın on ikinci bölümünün sonunda yer alan notlardan yararlanılarak, tezin konusuna ilişkin kısa bir literatür taraması sunulmuştur.

2024, 47 sayfa

Anahtar Kelimeler: Regüler tamamlama, Kordal graflar, Pozitif tanımlı tamamlama

PREFACE AND ACKNOWLEDGEMENTS

This thesis is a review study, and the main source used in its preparation is "Graphs and Matrices", Bapat (2014). In order for this book to be the main source for the thesis, my first advisor Asst. Prof Dr. Celalettin KAYA has communicated with the author Ravindra B. Bapat via e-mail, and he has received the following reply: “I am pleased that you and your students found my book useful. You may use the book for the thesis, subject to copyright laws. There is a close connection between graph theory and matrix theory. Techniques in matrix theory can be fruitfully used in graph theory. But this connection is ignored to a large extent by graph-theorists. Perhaps the reason is that graph theory is introduced as a part of combinatorics and not as algebra/linear algebra. There are many examples of linear algebra techniques in graph theory. The recent proof of the sensitivity conjecture by Huang is a brilliant example of such applications. These were some of my motivations in writing the book. It seems that the book is well-received, particularly in China, Iran, etc. I wish your students best luck and success in their future endeavours in graphs and matrices.”

After the permission of the author, the mentioned book, which is one of the excellent books prepared at the graduate level in the intersection of linear algebra and graph theory, has been adopted as the main source of the thesis. Therefore, almost all definitions and theorems in the main chapter of the thesis have been taken from Bapat (2014), and instead of citing each one separately, it was found more convenient to state this situation here. Other resources are stated at the beginning of the related section.

After stating these, I would like to thank the first advisor of my thesis, Asst. Prof. Dr. Celalettin KAYA, for his patience, guidance, and understanding. Also, I extend my sincere thanks to my virtuous advisor, Asst. Prof. Dr. Hanife VARLI, thank you for accepting me as my thesis advisor and supporting me. As well as I would like to convey my gratitude to the head of the Department of Mathematics and the teaching team for their well-established scientific recommendations.

Zahraa Ihsan Abdulwahid ALSAUD
Çankırı-2024

CONTENTS

LIST OF SYMBOLS

Γ	A graph
$adj(M)$	Adjoint of a matrix M
Γ^c	Bipartite complement of a graph Γ
K_n	Complete graph on n vertices
C_n	Cycle on n vertices
$\det(M)$	Determinant of a matrix M
$E(\Gamma), E$	Edge set of a graph Γ
M_{ij}, m_{ij}	(i, j)-entry of a matrix M
$\Delta(\Gamma), \Delta$	Maximum vertex degree of a graph Γ
$M_{m\times n}$	M is an $m \times n$ matrix
$\mathcal{N}(M)$	Null space of a matrix M
$\text{rank}(M)$	Rank of a matrix M
M/X	Schur complement of X in M
Γ_M	Specification graph associated with a matrix M
$\Gamma[S]$	Subgraph of a graph Γ induced by a vertex set $S \subseteq V(\Gamma)$
$\Gamma - e, \Gamma \setminus e$	Subgraph of a graph Γ obtained by deleting $e \in E\ (\Gamma)$
$\Gamma - v, \Gamma \setminus v$	Subgraph of a graph Γ obtained by deleting $v \in V\ (\Gamma)$
$M_{m\times n}(i\|j)$	Submatrix of a matrix M obtained by deleting row i and column j
$M_{m\times n}\ (A\|B)$	Submatrix of a matrix M with row numbers in $A^c \subseteq [m]$ and column numbers in $B^c \subseteq [n]$
$M_{m\times n}[A\|B]$	Submatrix of a matrix M with row numbers in $A \subseteq [m]$ and column numbers in $B \subseteq [n]$
$0_{m\times n}$	The $m \times n$ zero matrix
$\bar{0}$	The $n \times 1$ zero vector
$[n]$	The set $\{1,2, \dots, n\}$ of positive integers
$\text{tr}(M)$	Trace of a matrix M
M^T	Transpose of a matrix M
$v_i \sim v_j$	Vertex v_i is adjacent to vertex v_j
$V(\Gamma), V$	Vertex set of a graph Γ

LIST OF ABBREVIATIONS

Iff	If and only if
NCG	Nonsingular completable graph
NC	Nonsingular completion
PPDM	Partial positive definite matrix
PPSDM	Partial positive semi-definite matrix
PSM	Partial symmetric matrix
PEO	Perfect elimination ordering
PEM	Perfect matching
PDCG	Positive definite completable graph
PDC	Positive definite completion
PDCP	Positive definite completion problem
PDM	Positive definite matrix
PSDCG	Positive semi-definite completable graph
PSDM	Positive semi-definite matrix
SG	Specification graph
s.t.	Such that
TFAE	The following are equivalent
∃!	There exists unique
Wrt	With respect to
Wlog	Without loss of generality
Γ-PAM	Γ-partial matrix

1. PRELIMINARIES: MATRIX THEORY BACKGROUND

In this preliminary chapter, we survey some essential notions from linear algebra and matrix theory to present a self-contained thesis. But of course, it is not possible to prepare a thesis including all the fundamental notions from these two areas. Therefore, we skip some very basic definitions and facts, and we do not give proof of many of the theorems. Omitted proofs related to linear algebra or matrix theory can be found in many undergraduate or graduate linear algebra or matrix theory textbooks.

1.1 Matrices

We consider usually real matrices, but sometimes we also include complex matrices. As it is known, in almost all cases, if a theorem in the real case holds, then the corresponding theorem does also hold in the complex case.

1.1.1 A few basic definitions

Definition 1.1 An “$m \times n$ matrix” is an arrangement of mn entries in m rows and n columns. If M is an $m \times n$ matrix, the entry in the intersection of the k th row and l th column is donated by m_{kl}, and we write $M = [m_{kl}]$. An $m \times 1$ (respectively, $1 \times n$) matrix is called a “column vector” (respectively, “row vector”). An $n \times n$ matrix is called a “square matrix (of order n)”.

Notation 1.1 The vector space of all $m \times n$ matrices over $\mathbb{R}$ (respectively, over $\mathbb{C}$) is denoted by $\mathbb{R}^{\mathrm{m\times n}}$ (respectively, $\mathbb{C}^{\mathrm{m\times n}}$).

Definition 1.2 Let $M_{n\times n} = \left[m_{ij}\right]$ be a square matrix. If $m_{kl} = 0$ for $k \neq l,$ then M is called a "diagonal matrix". A diagonal matrix with (main) diagonal entries $m_{11} = \mu_1, m_{22} = \mu_2, \dots, m_{nn} = \mu_n$ denoted by “diag($\mu_1, \mu_2, \dots, \mu_n$)’’; and if $\mu_i = 1$ for each i, M is called the "identity matrix (of order n) ", and it is denoted by I_n or (if its order is obvious) by I. If $m_{ij} = 0$ for each $i > j$ (respectively, $i < j$), then M is called an "upper triangular (respectively, "lower triangular") matrix. It is obvious that M is upper triangular iff M^T is lower triangular.

Definition 1.3 Let $M_{n\times n} = [m_{ij}]$ be a square matrix, then the "trace" and the "determinant", respectively denoted by $tr\ (M)$ and $\det(M)$, are defined as follows:

$$\mathrm{tr}(M) = \sum_{i=1}^{n} m_{ii}\,, \qquad \det(M) = \sum_{\tau\in S_n} sgn\ (\tau)\ m_{1\tau(1)}\ m_{2\tau(2)} \dots m_{n\tau(n)},$$

where the sum in the definition of the determinant taken over all permutations τ: $[n] \to [n]$, and sgn(τ) is $+1$ or -1 if τ is even or odd, respectively.

Note 1.1 From the definition of the trace, it is easy to see that $tr(MN) = tr(NM)$ for every $n \times n$ square matrices M and N.

1.1.2 Vector spaces related to a matrix

Notation 1.2 The vector space of column vectors (respectively, row vectors) with n components over $\mathbb{R}$ (or over $\mathbb{C}$), that is, the vector space of $n \times 1$ (respectively, $1 \times n$) matrices over $\mathbb{R}$ (or over $\mathbb{C}$) is denoted by $\mathbb{R}^n$ (respectively, $\mathbb{C}^n$) in both cases.

Definition 1.4 Let M be an $m \times n$ matrix and let $r_1, r_2, \dots, r_m$ (respectively, $c_1, c_2, \dots, c_n$) be the rows (respectively, columns of M). The vector subspace of $\mathbb{R}^n$ (respectively, $\mathbb{R}^m$) generated by $r_L, r_2, \dots, r_m$ (respectively, $c_1, c_2, \dots., c_n$) is called the "row space" (respectively, "column space") of the matrix M. It is a well-known fact that "the dimension of the row space = the dimension of the column space"; and this value is called the "rank" of the matrix M, denoted by rank (M).

Definition 1.5 Let M be a $m \times n$ matrix. The vector subspace $\{x\ \in\ \mathbb{R}^n \colon = \bar{0}\ \}$ of $\mathbb{R}^n$ is called the "null space" of M, and it is denoted by $\mathcal{N}(M)$. The dimension of this space is called the “nullity” of M. It is a well-known fact that rank(M) + nullity$(M) = n$, where n is the number of columns of M.

1.1.3 Regular (or nonsingular) matrices

Definition 1.6 Let M be a square matrix of order n. If rank $(M) = n$ (respectively, $rank(M) < n$), then M is called a "regular" or "non-singular" (respectively, "singular") matrix. If M is regular, then $\exists!$ matrix, denoted by M^{-1}, called the "inverse" of M s.t. $MM^{-1} = M^{-1}M = I$. It is a well-known fact that M is regular iff $det(M) \neq 0$.

Definition 1.7 Let $M = [m_{ij}]$ be a square matrix of order n. The "cofactor" of the entry m_{kl} is “$(-1)^{k+\ell}\det(M(k \mid \ell))$”, where $M(k \mid \ell)$ will be formally defined in the "submatrices and minors" subsection. The "adjoint" of M, denoted by adj$(M) = [a_{ij}]$, is the matrix s.t. $a_{ij} = (-1)^{j+i}\ \det\big(M(j \mid i)\big)$.

Definition 1.8 Let M be an $m \times n$ matrix. M has “full column rank” (respectively, “full row rank”) if the rank$(M) = n$ (respectively, rank$(M) = m$). It is a well–known fact that if M does have full column rank (respectively, full row rank), then it does have a left inverse (respectively, right inverse), that is, $\exists\ A_{n\times m}$ (respectively, $\exists\ B_{n\times m}$) s.t. $AM = I_n$ (respectively, $MB = I_m$). Also, if rank $(M) = r$, then there is a $m \times r$ (respectively, $r \times n$) matrix X (respectively, Y) having full column rank (respectively, full row rank) s.t. $XY = M$, and this representation is called a "rank factorization" of M. It is a well- known fact that if rank$(M) = r$, then there are regular matrices P and Q of orders m and n, respectively, s.t. $M = P\begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}Q$, and this representation of M is called its "rank canonical form".

1.2 Eigenvalues of Symmetric and Hermitian Matrices

1.2.1 Characteristic polynomial

Definition 1.9 Let M be a square matrix of order n. $\det(M-\mu I)$ or $\det(\mu I-M)$ is a degree n polynomial of μ, and it is called the "characteristic polynomial" of M. The polynomial equation $det(\mu I-M)=0$ is the "characteristic equation" of M. Since $deg(det(\mu I-M))=n$, the characteristic equation has (counting with multiplicity) n complex roots, and each of these roots is called an "eigenvalue" or a "characteristic value" of M. The multiplicity of a characteristic value (as a root of the characteristic equation) is the "algebraic multiplicity" of this characteristic value. Over $\mathbb{C}$, the characteristic polynomial can be expressed as a product of liner polynomials:

$$det(\mu I-M)=(\mu-\mu_1)(\mu-\mu_2)\ldots(\mu-\mu_n)$$

where of course μ_i is a characteristic value of M for each $i=1,2,\ldots,n$. The dimension of $\mathcal{N}(\mu_i I-M)$ is the "geometric multiplicity" of the characteristic value μ_i for each $i=1,2,\ldots,n$. (The geometric multiplicity of a characteristic value $\leq$ The algebraic multiplicity of this characteristic value.)

Theorem 1.1 Let M and N be $m\times n$ and $n\times m$ matrices respectively, and assume that $m\geq n$. Let A be an $n\times n$ matrix with characteristic values $\mu_1,\mu_2,\ldots,\mu_n$. Also, let $p(x)$ be the characteristic polynomial of A, and $q(x)$ be an arbitrary polynomial. Then:

a) The characteristic values of MN and NM are the same, except for the case that MN has also the characteristic value 0 with multiplicity at least $m-n$.

b) $\det(A)=\mu_1\mu_2\ldots\mu_n$.

c) $tr(A)=\mu_1+\mu_2+\cdots+\mu_n$.

d) The sum of all k-products (that is, a product consisting of k factors) of characteristic values of A is equal to the sum of all $k\times k$ principal minors (a principal minor is defined formally in the “determinant” section) of A. (Note that if $k=1$, then we get the fact stated in part (c).)

e) The characteristic values of $q(A)$ are $q(\mu_1), q(\mu_2), \dots, q(\mu_n)$.

f) $p(A) = 0$. (The Cayley-Hamilton Theorem.)

g) There is a unique monic polynomial, say $m(x)$, of the minimum degree s.t. $m(A) = 0$, and this polynomial is called the "minimal polynomial" of A. ■

1.2.2 Spectral theorem

Definition 1.10 Let M be an $n \times n$ matrix. If $M = M^T$ in the real case (respectively, $M^* = M$, where $M^* = \overline{M}^T$ in the complex case), then M is called a "symmetric" (respectively, "Hermitian") matrix.

Theorem 1.2 Let M be a symmetric matrix of order n in the real case (respectively, a Hermitian matrix of order n in the complex case). Then:

a) The characteristic values of M are all real numbers.

b) The algebraic multiplicity of a characteristic value of M is equal to the geometric multiplicity of this characteristic value.

c) There is an orthogonal (respectively, unitary) matrix Q s.t. QMQ^T (respectively, QMQ^*) $= diag(\mu_1, \mu_2, \dots, \mu_n)$, where μ_i is a characteristic value of M for each $i = 1,2, \dots, n$.

d) $rank(M)$ is the number of nonzero characteristic values of M counting with multiplicity. ■

1.3 Determinants

This section is prepared by using the textbook “Matrix Theory: From Generalized Inverses to Jordan Form”, by Piziak and Odell (2007) in which the omitted proofs can be found.

We first define a map from the column space (equivalently, the row space can also be used) of square matrices over $\mathbb{C}$ to $\mathbb{C}$.

Definition 1.11 Let $D: \mathbb{C}^{n\times 1} \times \ldots \times \mathbb{C}^{n\times 1}\ (n\ copies) \to \mathbb{C}$ be a map. If for each $i \in [n]$, D satisfies the following two properties:

a) $D\ (\ldots, [c \propto_i], \ldots) = c\ D\ (\ldots, [\propto_i], \ldots)$,

b) $D\ (\ldots, [\propto_i + \beta_i\ ], \ldots) = D\ (\ldots, [\propto_i], \ldots) + D\ (\ldots, [\beta_i], \ldots)$,

where $\propto_i, \beta_i \in\ \mathbb{C}^{n\times 1}$, then D is called an "n-linear" map. Moreover, if $D = 0$ whenever there are equal adjacent columns, then D is called "alternating". If D is both n-linear and alternating, then it is called a "determinant function".

Note 1.2 The part (b) of the previous definition does not say that $D(M+N) = D(M) + D(N)$. In fact, this is false for $n > 1$. Also, note that a determinant is a map from $\mathbb{C}^{n\times n}$ to $\mathbb{C}$.

It is very well-known that for each $n \in \mathbb{N}$, there exists a determinant function and it is unique if we determine its value at I_n, the $n \times n$ identity matrix. This famous fact can be seen by proving the following theorem.

Theorem 1.3 Let $D: \mathbb{C}^{n\times 1} \times \ldots \times \mathbb{C}^{n\times 1}\ (n\ copies) \to \mathbb{C}$ be a determinant function. Then:

a) If there is $\bar{0}$ in some component of the input, then $D = 0$.

b) For each $i \in [n]$, $D\ (\ldots, [\propto_i], [\propto_{i+1}), \ldots) = -D\ (\ldots, [\propto_{i+1}], [\propto_i], \ldots)$.

c) For each $i, j \in [n], i < j, D(\ldots, [\propto_i], \ldots, [\propto_j], \ldots) = -D(\ldots, [\propto_j], \ldots, [\propto_i], \ldots)$.

d) If $\propto_i = \propto_j$ for some $i \neq j \in [n]$, then $D = 0$.

e) For each $i, j \in [n], i < j,$ for each scalar $c \in \mathbb{C}$, we have:

$$D\ (\ldots, [\propto_i], \ldots, [\propto_j] \ldots) = D(\ldots, [\propto_i], \ldots . c[\propto_i] + [\propto_j], \ldots).$$

f) $D\left(\begin{bmatrix} m_{11} \\ m_{21} \\ \vdots \\ m_{n1} \end{bmatrix}, \begin{bmatrix} m_{12} \\ m_{22} \\ \vdots \\ m_{n2} \end{bmatrix}, \ldots, \begin{bmatrix} m_{1n} \\ m_{2n} \\ \vdots \\ m_{nn} \end{bmatrix}\right) = \sum_{\tau \in S_n} (sgn(\tau)\, m_{1\tau(1)} m_{2\tau(2)} \ldots m_{n\tau(n)}) D(I_n)$. ■

Note 1.3 Part (f) of the previous theorem implies that a determinant function is uniquely determined by its value at I_n. Let D_c be s.t. $D_c(I_n) = c$. Then $D_c = cD_1$.

Definition 1.12 D_1 (namely, $D(I_n) = 1$) is called "the determinant function", and it is denoted by "det". Therefore, by part (f) the previous theorem, for each $M \in \mathbb{C}^{n\times n}$, we have:

$$\sum_{\tau\in S_n} sgn(\tau)\, m_{1\tau(1)} m_{2\tau(2)} \dots m_{n\tau(n)}.$$

By using the formula for det stated in the previous definition or the abstract definition of a determinant function (especially, for part (c)), the following corollary can be proved easily:

Corollary 1.1 Let $M, N, Q \in \mathbb{C}^{n\times n}$ and assume that P is invertible. Also for $i, j \in [n], i \neq j$, let P_{ij} (respectively, $T_{ij}(c)$) be the matrix obtained from I_n by interchanging the i th and the j th columns/rows (respectively, by adding c multiple of the i th column/row to the j th column/row.) Then it is known form elementary liner algebra that $M\, P_{ij}/P_{ij}M$ (respectively $M\, T_{ij}(c)/T_{ij}(c)M$) is the matrix obtained from M by interchanging the i th and the j th columns/rows (respectively, by adding c multiple of the i th column/row to the j th column/row). Finally, let $c \in \mathbb{C}$ be a constant. Then:

a) If M is an upper or lower triangular matrix, then $det(M) = m_{11}\, m_{22} \dots m_{nn}$.
b) $det(M^T) = det(M)$.
c) $det(MN) = det(M)\, det(N)$.
d) $det(Q^{-1} MQ) = det(M)$.
e) $det(MP_{ij}) = \det(P_{ij}M) = -\det(M)$.
f) $det(MT_{ij}(c)) = det(T_{ij}(c)M) = det(M)$.
g) $det(cM) = c^n\, det(M)$. ■

1.3.1 Submatrices and minors

Definition 1.13 Let M be an $m \times n$ matrix over $\mathbb{C}$ (or over $\mathbb{R}$), i.e., $M \in \mathbb{C}^{m\times n}$ (or $M \in \mathbb{R}^{m\times n}$). A matrix N obtained from M by deleting some of its rows and/or columns is called a "submatrix" of M.

Definition 1.14 Let $M \in \mathbb{C}^{m\times n}$ be a square matrix over $\mathbb{C}$. A matrix N obtained from M by deleting the rows $i_1, i_2, \dots, i_k$ and the columns $i_1, i_2, \dots, i_k$ is called a "principal submatrix " of M. If $i_1 = n-(k-1), i_2 = n-(k-2), .., i_k = n-k$, then N is called a "leading principal submatrix" of M; that is, a $k \times k$ "leading principal submatrix" is a submatrix obtained by taking rows. $1,2, \dots., k$ and columns $1,2, \dots., k$.

Notation 1. 3 Let M $\in$ $\mathbb{C}^{m\times n}$ and let $A \subseteq [m], B \subseteq [M]$ be non-empty subsets. Then:
a) $M[\,A \mid B\,]$ denotes the submatrix of M consisting of rows and columns with row indices in A and column indices in B, respectively.
b) $M\,(\,A \mid B\,)$ denotes the submatrix of M consisting of rows and columns with row indices not in A and column indices not in B, respectively.

Definition 1.15 Let $M \in \mathbb{C}^{m\times n}$ and $k = \min\{m,n\}$. And Let $A, B \subseteq [k]$ be non-empty subsets with $|A| = |B|$. Then, $\det(M[\,A \mid B\,])$ is called a $k \times k$ "minor" of M (or the "(A,B)-minor" of M). If $A = B$, than $\det(M[\,A \mid B\,])$ is called a "principal minor" of M; and if $A = B = \{1,2, \dots, \ell\}$, where $\ell \le k$, then $\det(M[\,A \mid B\,])$ is called a "leading principal minor" of M.

1.3.2 The Cauchy-Binet theorem

The Cauchy-Binet theorem is a generalization of the very well-known fact that for any two square matrices M and N, $\det(MN) = \det(M)\det(N)$. We state it without proof.

Theorem 1.4 (Cauchy-Binet Theorem) Let $= \left[x_{ij}\right] \in \mathbb{C}^{m\times n}$, $Y = \left[y_{ij}\right] \in \mathbb{C}^{n\times p}$, and Z$=$ XY. Also, let $r = \min\{m, n, p\}$ and $s \in [r]$. Assume that $A \subseteq [m], B \subseteq [p]$ s.t. $|A| = |B| = s$. Then:

$$\det(Z[\,A \mid B\,]) = \textstyle\sum_{C\subseteq[n]} \det(X[A|C])\ \det(Y\,[C|B]),$$

where the summation is taken over all s-subsets of the set $[r]$. ∎

1.3.3 Laplace expansion theorem

The Laplace expansion theorem is a generalization of the well-known Laplace cofactor expansion theorem. It expresses the determinant of a square matrix wrt rows (or columns) and determinants of smaller-order square matrices. We state it without proof.

Notation 1.4 Let $A = \{j_1, j_2\,, \dots, j_k\} \subseteq [n]$. Then: $sum\ (A) = j_1 + j_2 + \cdots + j_k$.

Theorem 1.5 (Laplace Expansion Theorem) Let X be an $n \times n$ matrix and $A \subseteq [n]$ (respectively, $B \subseteq [n]$) with $|A| = k$ (respectively, $|B| = k$). Then:

a) (Fix A) $\det(X) = \sum_{\substack{B\subseteq[n]\\|B|=k}} (-1)^{sum\ (A)+sum\ (B)} \det(X[A|B]) \det\big(X(A|B)\big)$.

b) (Fix A) $\det(X) = \sum_{\substack{A\subseteq[n]\\|A|=k}} (-1)^{sum\ (A)+sum\ (B)} \det(X[A|B]) \det\big(X(A|B)\big)$. ∎

The usual Laplace cofactor expansion theorem is a particular case of the previous theorem, we just take $A = \{i\}$ in part (a) and $B = \{j\}$ in part (b).

There exists an amazing relation between determinants and inverses as stated in the next theorem.

Definition 1.16 Let M be an $n \times n$ matrix. The "(k,l)-cofactor" of M is the scalar $(-1)^{k+l} \det\big(M(\,k \mid l\,)\big)$. The "cofactor matrix" of M, denoted by $cof(M)$, is the matrix whose (k,l)-entry is the (k,l)-cofactor of M. The "adjoint" of M, denoted by $adj(M)$, is the matrix whose (k,l)-entry is $(-1)^{l+k} \det\big(M(\,l \mid k\,)\big)$, that is, $adj(M) = cof(M)^T$. (We take transpose to define the adjoint matrix because the following theorem is true in this case.)

Theorem 1.6 Let M be a square matrix of order n. Then:
a) $Madj(M) = adj(M)M = \det(M)\, I_n$.
b) M is invertible ⇔ $\det(M) \neq 0$. In this case, $M^{-1} = (det(M)^{-1}\, adj\ (M)$. ■

We complete this subsection with an important theorem related to the determinant of a partitioned matrix and a corollary of it, and these results are used frequently.

Theorem 1.7 For matrices X, $Y, Z, 0$ of suitable orders, we have:

$$det \begin{bmatrix} X & Y \\ 0 & Z \end{bmatrix} = \det(X)\, det(Z). \quad (*)$$

Proof. Fix matrices X and Y, and define a map $D(X,Y,Z) = det \begin{bmatrix} X & Y \\ 0 & Z \end{bmatrix}$ of the variable Z. Suppose that Z is an $n \times n$ matrix. (Of course, the equation $(*)$ is meaningful only if X and Z are square matrices of suitable orders.) Then D is an n-linear map of rows (columns) of Z and is alternating because the determinant is n-linear map of rows (columns) is alternating. Therefore, by uniqueness of determinants, we have:

$$D\ (X,Y,Z) = D\left(X, Y, \begin{bmatrix} z_{11} & z_{12} & \cdots & z_{1n} \\ z_{21} & z_{22} & \cdots & z_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \cdots & z_{nn} \end{bmatrix} \right)$$

$$= \left(\sum_{\tau \in S_n} sgn(\tau) z_{1\tau(1)} z_{2\tau(2)} \dots z_{n\tau(n)} \right) D(X,Y,I_n) = \det(Z) D(X,Y,I_n).$$

Now, if we multiply row j of I_n, say r_j, with $\left(-y_{ij}\right)$ and add $\left(-y_{ij}\right)r_j$ to the row i of Y, for each $i, j = 1,2, \ldots.., n$, then the obtained matrix will be the zero matrix. And the value of the determinant does not change by the corresponding property of the determinant. Therefore, $D(X, Y, I_n) = D(X, 0, I_n)$.

Assume that X is an $m \times m$ matrix. Then $D(X, 0, I_n) = \det \begin{bmatrix} X & 0 \\ 0 & I_n \end{bmatrix}$ is m-linear map of rows (and columns) of X and is alternating. Therefore, by uniqueness of the determinant, we have:

$$D\ (X, 0, I_n) = D\left(\begin{bmatrix} x_{11} & x_{11} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nn} \end{bmatrix}, 0, I_n\right)$$

$$= \left(\sum\nolimits_{\tau \in S_n} sgn(\tau) x_{1\tau(1)} x_{2\tau(2)} \ldots x_{n\tau(n)}\right) D(I_m, 0, I_n) = det(X)\ D(I_m, 0, I_n).$$

Then, since $D(I_m, 0, I_n) = det \begin{bmatrix} I_m & 0 \\ 0 & I_n \end{bmatrix} = 1, D(X, 0, I_n) = det(X)$.

$$\therefore det \begin{bmatrix} X & Y \\ 0 & Z \end{bmatrix} = D\ (X, Y, Z) = det(Z)\, D(X, Y, I_n) = det(Z)\, det(X). \blacksquare$$

Corollary 1.2 Let X, Y, Z, W be matrices of suitable orders. Then:

a) $det \begin{bmatrix} X & 0 \\ Y & Z \end{bmatrix} = det(X)\ \ det(Z)$.

b) Let $M = \begin{bmatrix} X & Y \\ Z & W \end{bmatrix}$, and assume that X is regular. Then:

$$det(M) = det(X)\, det(W - ZX^{-1}Y).$$

c) $det \begin{bmatrix} I & Y \\ Z & W \end{bmatrix} = det(W - YZ)\ \ and\ det \begin{bmatrix} I & Y \\ Z & I \end{bmatrix} = det(I - YZ)$.

Proof.

a) $det\begin{bmatrix} X & 0 \\ Y & Z \end{bmatrix} = det\begin{bmatrix} X & 0 \\ Y & Z \end{bmatrix}^T = det\begin{bmatrix} X^T & Y^T \\ 0 & Z^T \end{bmatrix}$

$$= det(X^T)\ det(Z^T) \text{ (By the previous theorem.)}$$

$$= det(X)\, det(Z).$$

b) $\begin{bmatrix} X & Y \\ Z & W \end{bmatrix} = \begin{bmatrix} I & 0 \\ CA^{-1} & I \end{bmatrix}\begin{bmatrix} X & Y \\ 0 & W - ZX^{-1}Y \end{bmatrix}$

$\Rightarrow det\begin{bmatrix} X & Y \\ Z & W \end{bmatrix} = det\begin{bmatrix} I & 0 \\ CA^{-1} & I \end{bmatrix} det\begin{bmatrix} X & Y \\ 0 & W - ZX^{-1}Y \end{bmatrix}$

$$= 1\ \mathrm{det}(X)\ det(W - ZX^{-1}Y) \text{ (By the previous theorem.)}$$

c) Since $X = I$ and $X^{-1} = I$, it is trivially obtained from part (b). ■

1.3.4 Schur complement

The notion of Schur complement is related to invertible blocks of a partitioned matrix. For motivation, let $M = \begin{bmatrix} x & y \\ z & w \end{bmatrix}$ be a 2×2 matrix and assume that $x \neq 0$. Then since x is invertible, we have:

$$\begin{bmatrix} x & y \\ z & w \end{bmatrix} \xrightarrow[(r_i \leftrightarrow i \text{ th row})]{(-zx^{-1})r_1 + r_2 \to r_2} \begin{bmatrix} x & y \\ 0 & w - zx^{-1}y \end{bmatrix} \xrightarrow[(c_j \leftrightarrow j \text{ th column})]{(-yx^{-1})c_1 + c_2 \to c_2} \begin{bmatrix} x & 0 \\ 0 & w - zx^{-1}y \end{bmatrix}.$$

Equivalently:

$$\begin{bmatrix} 1 & 0 \\ -zx^{-1} & 1 \end{bmatrix}\begin{bmatrix} x & y \\ z & w \end{bmatrix}\begin{bmatrix} 1 & -x^{-1}y \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} x & 0 \\ 0 & w - zx^{-1}y \end{bmatrix}.$$

Note that since $\begin{bmatrix} 1 & 0 \\ -zx^{-1} & 1 \end{bmatrix}$ and $\begin{bmatrix} 1 & -x^{-1}y \\ 0 & 1 \end{bmatrix}$ are invertible,

M is invertible $\Leftrightarrow \begin{bmatrix} x & 0 \\ 0 & w - zx^{-1}y \end{bmatrix}$ is invertible.

$\Leftrightarrow$ (Since $x \neq 0,$) $w - zx^{-1}y \neq 0$.

Note 1.4 Note also that $\det(M) = x\,(w - zx^{-1}y)(= xw - yz)$.

Similarly, if we assume that $w \neq 0$, then:

Since $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x & y \\ z & w \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} w & z \\ y & x \end{bmatrix}$,

M is invertible $\Leftrightarrow$ $\begin{bmatrix} w & z \\ y & x \end{bmatrix}$ is invertible.

$\Leftrightarrow$ (With exactly the same manner with different symbols) $x - y\,w^{-1}z \neq 0$.

Now, can we generalize this approach to block matrices? Yes, we can:

Definition 1.17 Let $M = \begin{bmatrix} X_{k\times k} & Y_{k\times m} \\ Z_{n\times k} & W_{n\times m} \end{bmatrix}$ (respectively, $M = \begin{bmatrix} X_{n\times m} & Y_{n\times k} \\ Z_{k\times m} & W_{k\times k} \end{bmatrix}$) be a partitioned matrix s.t. X (respectively, W) is invertible. Then, "Schur complement of X (respectively, W) in M" denoted by M/X (respectively, $M//W$), is defined by the matrix equation $M/X = W - ZX^{-1}Y$ (respectively, $M//W = X - YW^{-1}Z$).

Note 1.5 With exactly as in the 2×2 case, if X (respectively, W) is invertible, then we have the following part (a) (respectively, part (b)):

a) $\begin{bmatrix} X & Y \\ Z & W \end{bmatrix} \xrightarrow[(rb_i \leftrightarrow i \text{ th row block})]{(-ZX^{-1})rb_1 + rb_2 \to rb_2} \begin{bmatrix} X & Y \\ 0 & W - ZX^{-1}Y \end{bmatrix} \xrightarrow[(cb_j \leftrightarrow j \text{ th column block})]{(-YX^{-1})cb_1 + cb_2 \to cb_2}$
$\begin{bmatrix} X & 0 \\ 0 & W - ZX^{-1}Y \end{bmatrix}$.

Equivalently:

$$\begin{bmatrix} I & 0 \\ -ZX^{-1} & I \end{bmatrix}\begin{bmatrix} X & Y \\ Z & W \end{bmatrix}\begin{bmatrix} I & -X^{-1}Y \\ 0 & I \end{bmatrix} = \begin{bmatrix} X & 0 \\ 0 & W - ZX^{-1}Y \end{bmatrix}.$$

b) $\begin{bmatrix} X & Y \\ Z & W \end{bmatrix} \xrightarrow{(-YW^{-1})\, rb_2 + rb_1 \to rb_1} \begin{bmatrix} X - YW^{-1}Z & 0 \\ Z & W \end{bmatrix} \xrightarrow{(-ZW^{-1})\, cb_2 + cb_1 \to cb_1}$
$\begin{bmatrix} X - YW^{-1}Z & 0 \\ 0 & W \end{bmatrix}.$

Equivalently:

$$\begin{bmatrix} I & -YW^{-1} \\ 0 & I \end{bmatrix}\begin{bmatrix} X & Y \\ Z & W \end{bmatrix}\begin{bmatrix} I & -W^{-1}Z \\ 0 & I \end{bmatrix} = \begin{bmatrix} X - YW^{-1}Z & 0 \\ 0 & W \end{bmatrix}.$$

Theorem 1.8 (Schur (Complement) Formula) With the notation given in the previous definition, we have the following useful facts by the previous note:

a) $det(M) = det(X)\, det(W - ZX^{-1}Y) = det(X)\, det(M/X)$.

b) $det(M) = det(W)\, det(X - YW^{-1}Z) = det(W)\, det(M//W)$.

Note 1.6 From the previous theorem, we have:

a) If any two of $M, X, M/X$ are regular, then the third one is also regular.

b) If any two of $M, W, M//W$ are regular, then the third one is also regular.

Theorem 1.9 (Inverse of a Partitioned Matrix (Banacheiwichz Inversion Formula)) With the notation of the previous theorem, we have:

a) If X and M/X are regular, then M is also regular, and:

$$M^{-1} = \begin{bmatrix} X & Y \\ Z & W \end{bmatrix}^{-1} = \begin{bmatrix} X^{-1} + X^{-1}Y\,(M/X)^{-1}\,ZX^{-1} & -X^{-1}\,Y\,(M/X)^{-1} \\ -\,(M/X)^{-1}\,ZX^{-1} & (M/X)^{-1} \end{bmatrix}.$$

b) If W and $M//W$ are regular, then M is also regular, and:

$$M^{-1} = \begin{bmatrix} X & Y \\ Z & W \end{bmatrix}^{-1} = \begin{bmatrix} (M//W)^{-1} & -(M//W)^{-1}YW^{-1} \\ -W^{-1}Z\,(M//W)^{-1} & W^{-1} + W^{-1}Z(M//W)^{-1}YW^{-1} \end{bmatrix}.$$

Proof. We prove part (a), and part (b) can be proved with exactly the same manner. We prove by straightforward computation:

a) Let $\begin{bmatrix} X & Y \\ Z & W \end{bmatrix} \begin{bmatrix} X^{-1} + X^{-1}Y\,(M/X)^{-1}\,ZX^{-1} & -X^{-1}\,Y\,(M/X)^{-1} \\ -\,(M/X)^{-1}\,ZX^{-1} & (M/X)^{-1} \end{bmatrix} = \begin{bmatrix} \mathrm{A} & \mathrm{B} \\ \mathrm{C} & \mathrm{D} \end{bmatrix}$.

$$\begin{aligned}
A &= X\,(X^{-1} + X^{-1}Y\,(M/X)^{-1}\,ZX^{-1}) + Y(-\,(M/X)^{-1}\,ZX^{-1}) \\
&= I + Y(M/X)^{-1}ZX^{-1} - Y\,(M/X)^{-1}\,ZX^{-1} = I. \\
B &= X\,(-X^{-1}\,Y\,(M/X)^{-1}) + Y\,((M/X)^{-1}) = -Y\,(M/X)^{-1} + Y\,(M/X)^{-1} = 0. \\
C &= Z\,(X^{-1} + X^{-1}Y\,(M/X)^{-1}\,ZX^{-1}) + W\,(-(M/X)^{-1}ZX^{-1}) \\
&= ZX^{-1} + ZX^{-1}Y\,(M/X)^{-1}\,ZX^{-1} - W\,(M/X)^{-1}ZX^{-1} \\
&= ZX^{-1} + [(ZX^{-1}Y - W)(M/X)^{-1}]ZX^{-1} \\
&= ZX^{-1} + [-\,(M/X).\,(M/X)^{-1}]ZX^{-1} \\
&= ZX^{-1} - ZX^{-1} = 0. \\
D &= Z\,(-X^{-1}\,Y\,(M/X)^{-1}) + W\,((M/X)^{-1}) \\
&= -ZX^{-1}Y\,(M/X)^{-1} + W\,(M/X)^{-1} \\
&= (-ZX^{-1}Y + W)(M/X)^{-1} \\
&= (M/X)(M/X)^{-1} = I.
\end{aligned}$$

$\therefore \begin{bmatrix} A & B \\ C & D \end{bmatrix} = I$. $\therefore$ By the uniqueness of the inverse, the result is proved. ■

1.3.5 The Jacobi identity for determinants

We state the Jacobi identity for determinants without proof.

Theorem 1.10 (The Jacobi identity for determinants) Let X be a regular matrix of order n, and let $Y = X^{-1}$. Also let A, B be proper nonempty subsets of $[n]$ with $|A| = |B|$. Then:

$$\det\big(Y(A|B)\big) = \frac{1}{\det(X)}\det(X[B|A]) \cdot \blacksquare$$

1.4 Positive Semidefinite and Positive Definite Matrices

This section is prepared by using the textbook “Completely Positive Matrices”, by Berman and Shaked-Monderer (2021). In this section, we survey basic notions about PSDMs and PDMs in the real case, and we restrict ourselves mainly to the properties that are needed in the main chapter (Chapter 2) of the thesis.

Definition 1.18 Let M be an $n \times n$ matrix. If M is symmetric and $x^T M x \geq 0$ for every $x \in \mathbb{R}^n$, then M is called a "positive semidefinite matrix (PSDM)".

Proposition 1.1 Let M, N be PSDMs. X be an $n \times m$ matrix, $a > 0$ be a real number. Then:

a) $M + N$ is a PSDM.

b) aM is a PSDM.

c) $X^T M X$ is a PSDM.

d) Any principal submatrix of M is also a PSDM.

Proof. Let $x \in \mathbb{R}^n, y \in \mathbb{R}^m$ be arbitrary vectors.

a) $x^T\ (M + N)x = x^T M x + x^T M y \geq 0 + 0 = 0.$

b) $x^T (aM) x = a(x^T M x) \geq a0 = 0.$

c) $y^T\ (X^T M X) y = (y^T X^T)\ M\ (Xy) = (Xy)^T\ M\ (Xy) \geq 0.$

d) Let $A = \{1 \leq i_1 < i_2 < \cdots < i_k \leq n\} \subseteq [n]$ be an arbitrary subset, $z = \left[z_{i_1}, z_{i_2}, \dots, z_{i_k}\right]^T \in \mathbb{R}^k$ be an arbitrary vector. And let $w = [w_1, w_2 \dots, w_n]^T \in \mathbb{R}^n$ be the vector defined by $w_j = \begin{cases} z_{i_m}, & if\ j = i_m \in A, \\ 0, & if\ j \notin A. \end{cases}$

Then: $z^T M\ [A|A] z = w^T\ M w \geq 0.$ ■

Note 1.7 Let $M_{n\times n}$ be a PSDM. Then, since M is symmetric by definition; M does have n real characteristic values, counting with multiplicity, and M is orthogonally diagonalizable, i.e., there is an orthogonal matrix P s.t. $P^T M P = D$, a diagonal matrix. Therefore, $rank\ M = rank\ D =$ The number of nonzero characteristic values of M.

Now, we state and prove several characterizations of PSDMs. We first give a definition that is needed for one of these characterizations.

Definition 1.19 Let $x_1, x_2, \dots, x_n$ be vectors in a real inner product space W, with the inner product $<, >$. Then the matrix:

$$G = \begin{bmatrix} < x_1, x_1 > & < x_1, x_2 > & \dots & < x_1, x_n > \\ < x_2, x_1 > & < x_2, x_2 > & \cdots & < x_2, x_n > \\ \vdots & \vdots & \ddots & \vdots \\ < x_n, x_1 > & < x_n, x_2 > & \dots & < x_n, x_n > \end{bmatrix}.$$

is called the "Gram matrix" of the vectors $x_1, x_2, \dots, x_n$ and is denoted by $G(x_1, x_2, \dots, x_n)$.

Theorem 1.11 Let $M \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Then, TFAE:

a) M is a PSDM.

b) All the characteristic values of M are ≥ 0.

c) All the principal minors of M are ≥ 0.

d) There is a matrix $N \in \mathbb{R}^{n \times k}$ s.t. $M = NN^T$.

e) There is a lower triangular matrix $L \in \mathbb{R}^{n \times n}$ s.t. $M = LL^T$.

f) There is a symmetric matrix $P \in \mathbb{R}^{n \times n}$ s.t. $M = P^2$.

g) There is a k-dimensional real inner product space W, and vectors $x_1, x_2, \dots, x_n \in W$ s.t. $M = G\,(x_1, x_2, \dots, x_n)$.

h) There are k vectors $v_1, v_2, \dots, v_k \in \mathbb{R}^n$ s.t. $M = \sum_{j=1}^{k} v_j v_j^T$. ■

Proof. We demonstrate the implications: $(a) \Longrightarrow (b), (a) \Longrightarrow (c) \Longrightarrow (b) \Longrightarrow (f) \Longrightarrow (d) \Longrightarrow (g) \Longrightarrow (a), (d) \Longrightarrow (e) \Longrightarrow (d),$ and $(b) \Leftrightarrow (h)$:

$(a) \Longrightarrow (b)$: Let μ be a characteristic value of M, and x be a characteristic vector of M corresponding to μ. Then, $x \neq 0$, and $Mx = \mu x$. Now:

$Mx = \mu x \Rightarrow x^T Mx = x^T \mu x = \mu\, x^T x \Rightarrow$ Since $x^T Mx \geq 0$ and $x^T x > 0, \mu = \frac{x^T Mx}{x^T x} \geq 0$.

$(a) \Rightarrow$ (c): Let $A \subseteq [n]$. Consider the principal submatrix $M[A|A]$ of M. First, from the previous proposition, $M[A|A]$ is also a PSDM. Then, by $(a) \Rightarrow$ (b), all the characteristic values of $M[A|A]$ is ≥ 0. Therefore, since the determinant of a matrix is the product of all the characteristic values of the matrix, $\det M[A|A] \geq 0$.

$(c) \Rightarrow (b)$: Let $p_M(x) = \det(xI - M) = x^n - a_1x^{n-1} + a_2x^{n-2} - \cdots + (-1)^k\, a_k\, x^{b-k} + \cdots + (-1)^{n-1}a_{n-1}x + (-1)^{\mathrm{n}}a_n$ be the characteristic polynomial of M. Then since a_k is the sum of all the k-products of the characteristic values of M, a_k is equal to the sum of all the $k \times k$ principal minors of M. (It is a well-known fact that "the sum of all the k-products of the characteristic values of a matrix" = "the sum of all the $k \times k$ principal minors of M".) Therefore, since all the principal minors of M are ≥ 0 by the hypothesis, $a_k \geq 0$ for each $k = 1,2,\dots,n$.

Now, assume that $c < 0$.

Case 1. Assume that n is even. Then, $c^n > 0$. And $(-1)^k\, a_kc^{n-k} \geq 0$ for each $k = 1,2,\dots,n$:

k-even $\Rightarrow (-1)^k = 1$ and $(n-k)$-even $\Rightarrow (-1)^k\, a_k\, c^{n-k} \geq 0$.

k-odd $\Rightarrow (-1)^k = -1$ and $(n-k)$-odd $\Rightarrow (-1)^k\, a_k\, c^{n-k} = -a_k\, c^{n-k} \geq 0$.

$\therefore p_M(c) > 0$.

Case 2. Assume that n is odd. Then, $c^n < 0$. And $(-1)^k\, a_kc^{n-k} \leq 0$ for each $k = 1,2,\dots,n$:

k-even $\Rightarrow (-1)^k = 1$ and $(n-k)$-odd $\Rightarrow (-1)^k\, a_k\, c^{n-k} \leq 0$.

k-odd $\Rightarrow (-1)^k = -1$ and $(n-k)$-even $\Rightarrow (-1)^k\, a_k\, c^{n-k} = -a_k\, c^{n-k} \leq 0$.

$\therefore p_M(c) < 0$.

As a result of Case 1 and Case 2, $p_M(c)$ does not have any negative root. In other words, M does not have any negative characteristic value.

$\therefore$ Since all the characteristic values of M are real (because $M = M^T$), all the characteristic values of M are ≥ 0.

$(b) \Rightarrow (f)$: Since $M = M^T$ and since its characteristic values are all ≥ 0 by the hypothesis, there is an orthogonal matrix Q s.t. $Q^T\, M\, Q = D = diag(d_1, d_2, \dots, d_n)$, where $d_i \geq 0$ for each $i = 1,2,\dots,n$. Then, $M = QDQ^T$.

Let$\sqrt{D} = diag\left(\sqrt{d_1}, \sqrt{d_2}, \dots, \sqrt{d_n}\right)$.

Then, $M = QDQ^T = Q\sqrt{D}\sqrt{D}\,Q^T = \left(Q\,\sqrt{D}\,Q^T\right)\left(Q\,\sqrt{D}\,Q^T\right) = NN = N^2$, where $N = Q\sqrt{\mathrm{D}}\,Q^T$ is an $n \times n$ real symmetric matrix.

$(d) \Rightarrow$ (e): To prove this statement, we use a well-known fact from linear algebra, namely QR-factorization: "Let $A \in \mathbb{R}^{m\times n}$. Then, there are matrices Q and R s.t. the rows of Q are orthonormal and R is upper triangular s.t. $A = QR$". Assume that $M = NN^T$, where $N \in \mathbb{R}^{n\times k}$. Let $N^T = QR$ be a QR-factorization of N^T. Then:

$$M = NN^T = (QR)^T(QR) = R^T\,Q^TQR = R^TIR = R^TR.$$

$\therefore M = LL^T$, where $L = R^T$ is a lover triangular matrix.

$(d) \Rightarrow$ (g): Assume that $M = NN^T$ for some $n \times k$ real matrix N. Now, let $x_i = r_i^T$, where r_i is the i th row of N, and $W = \mathbb{R}^k$. Then, $x_i \in \mathbb{R}^k$ for each $k = 1,2,\dots,n$, because N has k columns. And $M = G(x_1, x_2, \dots, x_n)$:

$$M = NN^T = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{bmatrix} \begin{bmatrix} r_1^T & r_2^T & \dots & r_n^T \end{bmatrix} = \begin{bmatrix} r_1r_1^T & r_1\,r_2^T & \dots & r_1r_n^T \\ r_2\,r_1^T & r_2r_2^T & \dots & r_2r_n^T \\ \dots & \dots & \ddots & \dots \\ r_n\,r_1^T & r_nr_2^T & \dots & r_n\,r_n^T \end{bmatrix} = G(x_1, x_2, \dots, x_n),$$

because $g_{ij} < x_i, x_j > = x_i^T\,x_j = (r_i^T)^T\,r_j^T = r_ir_j^T = m_{ij}$, where $M = [m_{ij}]$ and $G(x_1, x_2, \dots, x_n) = [g_{ij}]$.

$(g) \Rightarrow (a)$: Let $[m_{ij}] = M = G(x_1, x_2, \dots, x_n)$, and let $y = [y_2, \dots y_n]^T \in \mathbb{R}^n$.Then:

$$y^T\,My = \sum_{i,j=1}^{n} m_{ij}\;y_i\,y_j = \sum_{i,j=1}^{n} < x_i,\; x_j > y_iy_j$$

$$= \sum_{i,j=1}^{n} < x_i\,y_i,\; x_jy_j > = < \sum_{i=1}^{n} x_i\,y_i, \sum_{j=1}^{n} x_j\,y_j >$$

$$= < \sum_{i=1}^{n} x_i\,y_i, \sum_{i=1}^{n} x_i\,y_i > = \left|\left|\sum_{i=1}^{n} x_i\,y_i\right|\right|^2 \geq\; 0.$$

$(b) \Leftrightarrow (h)$: First of all, since $(a) \Leftrightarrow (d)$; equivalently, we prove $(d) \Leftrightarrow (h)$:

$M = NN^T$, where $N \in \mathbb{R}^{n\times k}$.

$\Leftrightarrow M = [v_1\ v_2\ \dots\ v_k]\,, \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_k^T \end{bmatrix}$, where v_j is the j th column of N for each $i = 1,2,\dots,k$.

$\Leftrightarrow M = v_1v_1^T + v_2v_2^T + \dots + v_kv_k^T$ (By the block multiplication.) $\Leftrightarrow M = \sum_{j=1}^{k} v_jv_j^T$.

$(e) \Rightarrow (d)$: It is trivially true, just take $N = L$. (Note that the only restriction about the value of k is that k must be $\geq$ rank(M). Thus, for example, $k = n$ is possible.)
$(f) \Rightarrow (d)$: It is again trivially true, just take $N = P$. ■

Remark 1.1 The matrix N stated in part (d) of the previous theorem is not unique. Particularly, if rank$(M) = r$, then there is an $N \in \mathbb{R}^{n\times r}$ s.t. $M = NN^T$ (where of course, rank$(N) = r$):
First, since M is symmetric, there is an orthogonal matrix Q s.t. $Q^TMQ = D = diag(d_1, d_2, \dots, d_n)$. Since d_i's are the characteristic values of M, and since M is a PSDM, $d_i \geq 0$ for each $i = 1,2,..,n$. Also, since rank $(M) = r$, exactly r of its characteristic values are > 0. Say $d_i > 0$ for each $i = 1,2,\dots,r$. Now, $Q^TMQ = D \Rightarrow M = QDQ^T = Q\sqrt{D}\sqrt{D}\,Q^T = \left(Q\sqrt{D}\right)\left(Q\sqrt{D}\right)^T = \tilde{N}\tilde{N}^T$, where $[\tilde{n}_{ij}] = \tilde{N} = Q\sqrt{D}$. Note that since $d_j = 0$ for each $j = r+1\,, r+2\,, \dots, n$, $\tilde{n}_{ij} = 0$ for $i = 1,2,\dots,n$ and $and\ \ j = r+1\,, r+2\,, \dots, n$. Therefore, $\tilde{N}[\,1,2,\dots,n \mid r+1\; r+2\,, \dots, n\,] = 0$.
Finally, let $N = \tilde{N}\,[1,2,..,n|1,2,..,r]$. Then, $NN^T = M$:

$$M = \tilde{N}\tilde{N}^T = [N \mid 0]\left[\frac{N^T}{0}\right] = N\tilde{N} + 00 = N\tilde{N} \text{ (By the block multiplication).}$$

Unlike the matrix N stated in part (d) of the previous theorem, the PSDM P constructed in the proof of part (f) is unique:

Theorem 1.40 Let M be a PSDM. Then, there exists a unique PSDM P s.t. $P^2 = M$.

Proof. (This proof is taken from Zhang (2011).)

We proved the existence part in the previous theorem, but we want to prove it again with a different approach.

Existence. First of all, an n-square matrix can be considered as a linear operator on $\mathbb{C}^n$. By the spectral theorem, there are orthonormal characteristic vectors, say $x_1, x_2, \dots, x_n$, corresponding to the characteristic values, say $\mu_1, \mu_2, \dots, \mu_n$, respectively.

Then $\mathcal{B} = \{x_1, x_2, \dots, x_n\}$ is an orthonormal basis of $\mathbb{C}^n$, and $M(x_i) = \mu_i x_i$, $\mu_i \geq 0$, for each $i = 1,2, \dots, n$.

Define a linear operator $P\colon \mathbb{C}^n \to \mathbb{C}^n$ s.t. $P(x_i) = \sqrt{\mu_i}\, x_i$ for each $i = 1,2, \dots, n$. Then, for each $i = 1,2, \dots, n$, we have:

$$P^2(x_i) = P\left(P(x_i)\right) = P\left(\sqrt{\mu_i} x_i\right) = \sqrt{\mu_i}\, P(x_i) = \sqrt{\mu_i}\left(\sqrt{\mu_i} x_i\right) = \mu_i x_i = M(x_i).$$

∴ Since M and P^2 agree on a basis, $M = P^2$.

And P is also a PSDM: Let $x \in \mathbb{C}^n$ be an arbitrary vector, and let $x = a_1 x_i + a_2 x_2 + \cdots + a_n x_n$, where $a_i \in \mathbb{C}^n$. Then:

$$x^* P x = \left(\textstyle\sum_{i=1}^n a_i x_i\right)^* P \left(\textstyle\sum_{i=1}^n a_i x_i\right) = \left(\textstyle\sum_{i=1}^n \bar{a}_i x_i^*\right)\left(\textstyle\sum_{i=1}^n a_i P\,(x_i)\right)$$

$$= \left(\textstyle\sum_{i=1}^n \bar{a}_i x_i^*\right).\left(\textstyle\sum_{i=1}^n a_i \mu_i x_i\right)$$

$$= \textstyle\sum_{i=1}^n \bar{a}_i a_i \mu_i\, x_i^* x_i \text{ (Since } \mathcal{B} \text{ is an orthonormal basis, } x_i^* x_j = 0 \text{ for each } i \neq j.)$$

$$= \sum_{i=1}^n |a_i|^2\, \mu_i \left\|x_i\right\|^2 \geq 0.$$

∴ P is a PSDM.

Uniqueness. Assume that Q is also a PSDM s.t. $Q^2 = M$.

First, if x is a characteristic vector of Q, then $Qx = \mu x$ for some $\mu \geq 0$, where of course μ is a characteristic value of Q. And:

$$M(x) = Q^2(x) = Q\left(Q(x)\right) = Q(\mu x) = \mu Q(x) = \mu(\mu x) = \mu^2 x.$$

$\therefore M(x) = \mu^2 x$, that is, μ^2 is a characteristic value of M.

$\therefore$ The characteristic values of Q are the nonnegative square roots of the characteristic values of M.

$\therefore$ The characteristic values of Q are: $\sqrt{\mu_1}, \sqrt{\mu_2}, \dots, \sqrt{\mu_n}$.

Now, let $y_1, y_2, \dots, y_n$ be orthonormal characteristic vectors of Q corresponding to the characteristic values $\sqrt{\mu_1}, \sqrt{\mu_2} \dots, \sqrt{\mu_n}$, respectively.

Then $\mathcal{C} = \{y_1, y_2, \dots, y_n\}$ is an orthonormal basis of $\mathbb{C}^n$.

And let $x_j = a_{ij} y_i + a_{2j} y_2 + \cdots + a_{nj} y_n = \sum_{i=1}^{n} a_{ij} y_i$ for each $j = 1,2, \dots, n$. Then:

$$i)\ Q^2(x_j) = M(x_j) = \mu_j x_j = \textstyle\sum_{i=1}^{n} a_{ij}\, \mu_j\, y_i, \text{ and;}$$

$$ii)\ Q^2(x_j) = Q\left(Q(x_j)\right) = Q\left(Q\left(\textstyle\sum_{i=1}^{n} a_{ij} y_i\right)\right) z = Q\left(\textstyle\sum_{i=1}^{n} a_{ij}\, Q(y_i)\right)$$

$$= Q\left(\textstyle\sum_{i=1}^{n} a_{ij}\ \sqrt{\mu_i} y_i\right) = \textstyle\sum_{i=1}^{n} a_{ij}\ \sqrt{\mu_i}\, Q(y_i)$$

$$= \textstyle\sum_{i=1}^{n} a_{ij}\ \sqrt{\mu_i}\sqrt{\mu_i}\, y_i = \textstyle\sum_{i=1}^{n} a_{ij}\, \mu_i\, y_i.$$

$\therefore$ Since is $\mathcal{C}$ a basis, $a_{ij} \mu_j = a_{ij}\, \mu_i$ for each $i = 1,2, \dots, n$.

$\therefore a_{ij} \sqrt{\mu_j} = a_{ij} \sqrt{\mu_i}$ for each $i = 1,2, \dots, n$.

($a_{ij}\, \mu_j = a_{ij}\, \mu_i \Rightarrow$"If $a_{ij} = 0$, then $a_{ij}\sqrt{\mu_j} = a_{ij}\sqrt{\mu_i}$" and "if $a_{ij} \neq 0$, then $\mu_j = \mu_i$, thus $\sqrt{\mu_{\boldsymbol{j}}} = \sqrt{\mu_i}$. Hence $a_{ij}\sqrt{\mu_i} = a_{ij}\sqrt{\mu_i}$".)

Therefore, for each $j = 1,2, \dots, n$, we have:

$$Q(x_j) = Q\left(\textstyle\sum_{i=1}^{n} a_{ij}\, y_i\right) = \textstyle\sum_{i=1}^{n} a_{ij}\ Q(yi) = \textstyle\sum_{i=1}^{n} a_{ij}\ \sqrt{\mu_i}\, y_i$$

$$= \textstyle\sum_{i=1}^{n} a_{ij} \sqrt{\mu_j}\ y_i = \sqrt{\mu_i}\ \textstyle\sum_{i=1}^{n} a_{ij}\ y_i = \sqrt{\mu_i}\, x_j = P(x_j).$$

$\therefore$ Since $\mathcal{C}$ is a basis, $Q = P$. ■

Definition 1.20 Let M be a PSDM. The unique PSDM N satisfying $N^2 = M$ is called the "square root" of M, and it is denoted by $M^{1/2}$ or $\sqrt{M}$.

PSDMs have lots of interesting properties, and Bermen and Shaked-Monderer (2003) or (at an advanced level) Horn and Johnson (2012) are good references on this topic. We want to mention just one more property of PSDMs.

Proposition 1. 2 Let $M = [m_{ij}]$ be a PSDM. If $m_{ii} = 0$ for some $i \in \{1, 2, \dots, n\}$, then the i th row and the i th column of M are identically equal to zero.

Proof. Consider the principal submatrix $M\,[i,j|i,j] = \begin{bmatrix} m_{ii} & m_{ij} \\ m_{ji} & m_{jj} \end{bmatrix}$ for each $j = 1,2,..n$. Since M is a PSDM, the corresponding principal minor of M is ≥ 0, and since M is symmetric, we have:

$$\det \begin{bmatrix} m_{ii} & m_{ij} \\ m_{ji} & m_{jj} \end{bmatrix} = m_{ii}m_{jj} - m_{ij}\,m_{ji} = 0.\ m_{jj} - m_{ij}^2 = -m_{ij}^2 \geq 0.$$

$\therefore\ m_{ij} = 0$ for each $j = 1,2, \dots, n$.
$\therefore$ The i th row of M, and since M is symmetric, the i th column of M is identically equal to zero. ■

Definition 1.21 Let M be an $n \times n$ matrix. If M is symmetric and $x^T M x > 0$ for every nonzero $x \in \mathbb{R}^n$, then M is called a "positive definite matrix (PDM)".

Proposition 1.3 Let M be an $n \times n$ matrix. Then, M is a PDM iff M is a regular PSDM.

Proof.
($\Rightarrow$) Let $0 \neq x \in \mathbb{R}^n$. Then since M is a PDM, $x^T M x > 0$. Therefore, $x^T M x \geq 0$ for every $x \in \mathbb{R}^n$ (including the zero vector). Also, M is regular:

Suppose not. Then, there is a nonzero $x \in \mathbb{R}^n$ s.t. $Mx = 0$. But then $x^T Mx = x^T 0 = 0$, which contradicts with the positivity of M.

$\therefore$ M must be regular.

($\Leftarrow$) Since M is a PSDM, there is an $n \times r$ matrix N s.t. $M = NN^T$, where $r = rank(M)$. Then:

$$x^T Mx = x^T (NN^T)x = (x^T N)(N^T x) = (N^T x)^T (N^T x) = \left||N^T x|\right|^2.$$

Now, since $M = NN^T$, the null space $\mathcal{N}(M)$ of M is equal to the null space $\mathcal{N}(N^T)$ of N^T. ($\mathcal{N}(M) = \mathcal{N}(N^T)$ is proved in the next to last proposition of this section.)

$\therefore$ Since $x^T Mx = \left||N^T x|\right|^2, x^T Mx = 0$ iff $\left||N^T x|\right|^2 = 0$ iff $N^T x = 0$ iff $x \in \mathcal{N}(M)$.

$\therefore$ Since M is regular, that is, since $\mathcal{N}(M) = \{0\}$, $x^T Mx = 0$ iff $x = 0$.

$\therefore$ $x^T Mx > 0$ for every nonzero $x \in \mathbb{R}^n$.

$\therefore$ M is a PDM. ■

Now, we state (without proof) several characteristics of PDMs, which is analogous to the first theorem of this section characterizing PSDMs. But the next theorem has an additional characterization related to nested minors. Thus, we first define nested minors.

Definition 1.22 Let M be an $n \times n$ matrix. Let $A_i \subseteq [n]$ for each $i = 1,2,\dots,k$ s.t. $|A_i| = i$ and $A_i \subseteq A_{i+1}$. Then the minors $\det(M[A_i|A_i])$ are called "nested principal minors" of M. (Note that the leading principal minors $\det(M[1,2,\dots,i|1,2,\dots,i]), i = 1,2,\dots,n$, are n nested minors of M.)

Theorem 1.12 Let $M \in \mathbb{R}^{n\times n}$ be a symmetric matrix. Then, TFAE:

a) M is a PDM.

b) All the characteristic values of M are > 0.

c) All the principal minors of M are > 0.

d) There is a regular matrix $N \in \mathbb{R}^{n\times n}$ s.t. $M = NN^T$.

e) There is a regular lower triangular matrix $L \in \mathbb{R}^{n\times n}$ s.t. $M = LL^T$.

f) There is a regular symmetric matrix $P \in \mathbb{R}^{n\times n}$ s.t. $M = P^2$.

g) There is an n-dimensional real inner product space W, and linearly independent vectors $x_1, x_2, \dots, x_n$ s.t. $M = G(x_1, x_2, \dots, x_n)$.

h) There are n linearly independent vectors $v_1, v_2, \dots v_n \in \mathbb{R}^{n\times n}$ s.t. $M = \sum_{j=1}^{n} v_j v_j^T$.

i) There are n positive nested principal minors of M. ■

The previous theorem (except for the implication (i) $\Rightarrow (b)$) can be proved easily by using the characterization theorem of PSDMs (the first theorem of this section), the previous proposition, and the following result from linear algebra. The implication $(i) \Rightarrow (b)$ needs extra theory including an interlacing theorem. (The equivalent two versions of an interlacing theorem are given in Horn and Johnson (2012).)

Proposition 1.4 Let N be an $n \times k$ matrix and $M = NN^T \in \mathbb{R}^{n\times n}$. Then:

$$\mathcal{N}(M) = \mathcal{N}(N^T) \text{ and } CS(M) = CS(N),$$

where $\mathcal{N}$ denotes the null space and CS denotes the column space.

Proof.

Step 1. $\mathcal{N}(M) = \mathcal{N}(N^T)$:

$(\subseteq)$ $x \in \mathcal{N}(M = NN^T) \Rightarrow NN^T x = 0 \Rightarrow x^T NN^T x = 0 \Rightarrow (N^T x)(N^T x) = 0$

$$\Rightarrow \left|\left|N^T x\right|\right|^2 = 0 \Rightarrow N^T x = 0 \Rightarrow x \in \mathcal{N}(\mathrm{N}^\mathrm{T}).$$

$(\supseteq)$ $x \in \mathcal{N}(N^T) \Rightarrow N^T x = 0 \Rightarrow NN^T x = 0 \Rightarrow Mx = 0 \Rightarrow x \in \mathcal{N}(M)$.

$\therefore \mathcal{N}(M) = \mathcal{N}(N^T)$.

Step 2. First of all, since $\mathcal{N}(M) = \mathcal{N}(N^T)$, nullity($M$) = nullity($N^T$).

∴ Since rank+nullity = the number of columns, rank(M) = rank(N^T).

∴ Since rank(N) = rank(N^T), rank(M) = rank(N).

Secondly, $CS(M) \subseteq CS\ (N)$:

$y \in CS(M = NN^T) \Rightarrow NN^T x = y$ for some $x \in \mathbb{R}^n$.

$\Rightarrow N(N^T x) = y$, where $N^T x \in \mathbb{R}^k \Rightarrow$ Say $z = N^T x, Nz = y$.

$\Rightarrow y \in CS(N)$.

∴ Since rank(M) = rank(N), $CS(M) = CS(N)$. ■

Remark 1.2 An analogous statement to $(i) \Rightarrow (a)$ of the previous theorem is not true for PSDMs. That is, n nested principal minors of a matrix may be ≥ 0, but this matrix may not be a PSDM. For example, the two leading principal minors (which are two nested principal minors) of $M = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}$ are $M_1 = [0]$ and $M_2 = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}$, and $\det(M_1) = 0 \geq 0$, $\det(M_2) = 0 \geq 0$, but M is not a PSDM:

Let $x = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \in \mathbb{R}^2$. Then $x^T M x = [0\ 1] \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = [0\ 1] \begin{bmatrix} 0 \\ -1 \end{bmatrix} = -1 < 0$.

In spite of the previous remark, there is a weaker result for PSDMs, which is analogous to the implication $(i) \Rightarrow (a)$ of the previous theorem. We state it without proof:

Proposition 1.5 Let $M \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Assume that for $i = 1,2,\dots,n$, $\det(M[A_i|A_i])$ are nested principal minors of M s.t. for $i = 1,2,\dots,n-1$, $\det(M\,[A_i|A_i]) > 0$ and $\det(M)\,(= \det(M[1,2,\dots,n\,|1,2,\dots,n])) \geq 0$. Then M is a PSDM. ■

Note 1.8 Let M be a PSDM. Then, $\forall\ \varepsilon > 0, M + \varepsilon\mathrm{I}$ is a PDM:

μ is a characteristic value of $M \Leftrightarrow \det(\mu I - M) = 0$

$$\Leftrightarrow \det\left((\mu + \varepsilon) - \varepsilon)\, I - M\right) = 0$$

$$\Leftrightarrow \det\big((\mu + \varepsilon)I - \varepsilon I - \mu\big) = 0$$

$$\Leftrightarrow \det\big((\mu + \varepsilon)I - (\mu + \varepsilon I)\big) = 0$$

$\Leftrightarrow\ \mu + \varepsilon$ is a characteristic value of $M + \varepsilon I$.

Now since M is PSDM, all the characteristic values, say $\mu_1, \mu_2, \dots, \mu_n$ of M are ≥ 0.

$\therefore$ All the characteristic values, which are $\mu_1 + \varepsilon, \mu_2 + \varepsilon, \dots, \mu_n + \varepsilon$, of $M + \varepsilon I > 0$.

$\therefore M$ is a PDM by the previous theorem.

As a result of this observation, we obtain the following result:

Each PSDM is a limit of PDMs. The converse of this statement also holds: A matrix M which is a limit of PDMs (or PSDMs) is a PSDM.

We complete this section with a trivial proposition related to PDMs and Schur complements:

Proposition 1.6 Let $M = \begin{bmatrix} X & Y \\ Z & W \end{bmatrix}$ be a partitioned matrix, where X is a $k \times k$ square matrix. Then:

a) If M is a PDM, the Schur complement of X in M, namely $M/X = W - ZX^1Y$ is a PDM.

b) Let M be a symmetric matrix. If X and its Schur complement $M/X = W - ZX^{-1}Y$ are both PDMs, then M is a PDM.

Proof. First of all, from the Schur complement subsection, we know that:

$$\begin{bmatrix} I & 0 \\ -ZX^{-1} & I \end{bmatrix} \begin{bmatrix} X & Y \\ Z & W \end{bmatrix} \begin{bmatrix} I & -X^{-1}Y \\ 0 & I \end{bmatrix} = \begin{bmatrix} X & 0 \\ 0 & M/X \end{bmatrix}.$$

a) First, since M is a PDM, it is symmetric by definition. Therefore, $Z = Y^T$ and W is also a square matrix of order, say $(n-k) \times (n-k)$.

Second, since M is a PDM, all the principal minors of M are > 0. Therefore, since any principal minor of X or W is a principal matrix of M, all the principal minors of X and W are > 0. And thus, both X and W are PDMs. In particular, both X and W are symmetric and invertible.

Now, say $N = \begin{bmatrix} I & 0 \\ -ZX^{-1} & I \end{bmatrix} = \begin{bmatrix} I & 0 \\ -Y^TX^{-1} & I \end{bmatrix}$. Then:

$$N^T = \begin{bmatrix} I & (-Y^TX^{-1})^T \\ 0 & I \end{bmatrix} = \begin{bmatrix} I & -(X^{-1})^T(Y^T)^T \\ 0 & I \end{bmatrix} = \begin{bmatrix} I & -X^{-1}Y \\ 0 & I \end{bmatrix},$$

because $(X^{-1})^T = (X^T)^{-1}$ and $X^T = X$.

Also, $\det(N) = 1$ and thus N is a regular matrix. In fact:

$$N^{-1} = \begin{bmatrix} I & 0 \\ -ZX^{-1} & I \end{bmatrix}^{-1} = \begin{bmatrix} I & 0 \\ ZX^{-1} & I \end{bmatrix}.$$

$\therefore NMN^T$ is a PDM:

Obviously, NMN^T is symmetric. Let $0 \neq x \in \mathbb{R}^n$. Then:

$x^T NMN^T x = (N^T x)^T M(N^T x)$. And, say $y = N^T x$. Then, since N is regular and $x \neq 0$, $y \neq 0$.

$\therefore x^T(NMN^T)x = y^T My > 0$, because $y \neq 0$ and M is a PDM.

$\therefore NMN^T$ is a PDM. (In fact, the converse statement is also true.)

$\therefore$ Since a block diagonal matrix is a PDM iff each diagonal block is a PDM, (X is a PDM, which we already know, and) $M/X = W - ZX^{-1}Y = W - Y^T X^{-1} Y$ is a PDM.

b) First, since M is symmetric, $Z = Y^T$ and W is also a square matrix.

Second, $N = \begin{bmatrix} I & 0 \\ -Y^T X^{-1} & I \end{bmatrix}$ is invertible and $N^{-1} = \begin{bmatrix} I & 0 \\ Y^T X^{-1} & I \end{bmatrix}$. Therefore,

$$M = N^{-1} \begin{bmatrix} X & 0 \\ 0 & M/X \end{bmatrix} (N^{-1})^T.$$

Third, since X and M/X are PDMs, $\begin{bmatrix} X & 0 \\ 0 & M/X \end{bmatrix}$ is also a PDM. Therefore as part (a), $N^{-1} \begin{bmatrix} X & 0 \\ 0 & M/X \end{bmatrix} (N^{-1})^T$ is a PDM. ■

2. POSITIVE DEFINITE COMPLETION PROBLEM (PDCP)

There are many problems in various fields of mathematics related to completion problems. In particular, matrix theory has lots of completion problems, and it is very convenient to combine matrix theory and graph theory to struggle with such problems. In this main chapter of the thesis, we study one of the famous completion problems, namely, “positive definite completion problem (PDCP)”.

2.1 Nonsingular Completion (NC)

In this section, we briefly review the completion problem for matrices.

Definition 2.1 Let Γ be a bipartite graph with partite sets U and W s.t. $U = (u_1, u_2, \ldots, u_n)$ and $W = (w_1, w_2, \ldots, w_n)$ (note that the vertex sets U and W are considered as n-tuples). A square matrix $M = [m_{ij}]$ of order n, whose rows (respectively, columns) are indexed by U (respectively, W), is called a "Γ-partial matrix ($\Gamma -$ PAM)" if "m_{ij} is assigned a real number iff $u_i \sim w_j$". Let $S = \{\, (i,j) \mid m_{ij}$ is not assigned a real number$\}$. Then, an assignment $\varphi: S \to \mathbb{R}$ is called a "completion of the $\Gamma -$ PAM M". If any $\Gamma -$ PAM M has an NC (that is, if it is possible to assign real numbers to the remaining empty entries of M s.t. the obtained matrix is regular), then Γ is called a "nonsingular completable graph (NCG)".

Example 2.1 Let Γ be the bipartite graph with partite sets $U = (u_1, u_2, u_3)$ and $W = (w_1, w_2, w_3)$, and $E\,(\Gamma) = \big\{\{u_1, w_1\}, \{u_1, w_2\}, \{u_2, w_2\}, \{u_3, w_1\}, \{u_3, w_3\}\big\}$. And consider the following $\Gamma -$ PAM:

$$M = \begin{bmatrix} 1 & \sqrt{2} & ? \\ ? & -1 & ? \\ \pi & ? & 8 \end{bmatrix}.$$

Then, we can assign real numbers to the remaining empty entries (denoted by “?”) s.t. the resulting matrix is regular. For example:

$$N = \begin{bmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & -1 & 0 \\ \pi & 0 & 8 \end{bmatrix}.$$

is an NC of M. (It can be seen easily that $\det(N) = \pi - 24 \neq 0$, and thus N is regular). In fact, any $\Gamma - \text{PAM}$ has an NC: Let

$$M = \begin{bmatrix} a & b & x \\ y & c & z \\ d & t & e \end{bmatrix}$$

be a given $\Gamma - \text{PAM}$, where a, b, c, d, e are known real numbers, and x, y, z, t are empty entries which we will determine to get a regular matrix. Now, for example, choose $x = y = 1, z = 0$. To determine t: Let $s, u \in \mathbb{R}$ s.t. $sa + u1 = d$. Then choose a real number $t \neq sb + uc$. As a result, the obtained matrix N is regular, because (x, y, z, t are chosen in such a way that) the rows of N are linearly independent. ($m_{13} = 1, m_{23} = 0$. Therefore, row 1 and row 2 of N are linearly independent. And any linear combination of row 1 and row 2 is not equal to row 3. Therefore, $\{row1\ , row\ 2, row3\}$ is a linearly independent set of vectors).
∴ Γ is an NCG.

Definition 2.2 Let Γ be a bipartite graph with partite sets $U = (u_1, u_2, \ldots., u_n)$ and $W = (w_1, w_2, \ldots, w_n)$. Let Γ^c be the bipartite graph with the partite sets U and W s.t. $u_i \sim w_j$ in Γ^c (that is, $\{u_i, w_j\} \in E\ (\Gamma^c)$) iff $u_i \nsim w_j$ in Γ (that is $\{u_i, w_j\} \notin E\ (\Gamma)$). Then Γ^c is called the "bipartite complement" of the graph Γ.

Now, we characterize NCGs:

Theorem 2.1 Let Γ be a bipartite graph with partite sets

$$U = (u_1, u_2, \dots, u_n) \text{ and } W = (w_1, w_2, .., w_n).$$

Then: Γ is an NCG $\Leftrightarrow$ Γ^c has a "perfect matching (PEM)".

Proof.

($\Leftarrow$) Let $F = \left\{\left\{u_i, w_{\tau(i)}\right\} \mid i \in [n]\right\}$ $\left(\subseteq E\,(\Gamma)\right)$ be a PEM of Γ^c, where τ: $[n] \to [n]$ is a permutation. Let M be a $\Gamma -$ PAM. First of all, since $\left\{u_i, w_{\tau(i)}\right\} \in E(\Gamma^c), \left\{u_i, w_{\tau(i)}\right\} \notin E(\Gamma)$. Therefore, $\left(i, \tau(i)\right) -$entries of M are in the set S of empty entries of M. Let $M(z)$ be the matrix gotten from M as follows:

$$\left(M(z)\right)_{ij} = \begin{cases} z, & if\ j = \tau(i); \\ 0, & if\ (i,j) \in S \setminus \{(i, \tau(i) \mid i \in [n]\}. \end{cases}$$

Then, $\det M(z)$ is a polynomial in z of deg($\det M\,(z)$) $= n$ (with the leading coefficient ± 1). Therefore, counting with multiplicity, there are exactly n roots of $\det M(z)$ over $\mathbb{C}$. Thus, we can choose a real number z_0 s.t. $\det M(z_0) \neq 0$. That is, $M(z_0)$ is regular. Therefore, Γ is an NCG.

($\Rightarrow$)We prove this direction by its contrapositive: "Γ^c has no PEM $\Longrightarrow$ Γ is not an NCG". So, assume that Γ^c has no PEM. Then, there is a vertex cover V_c with $|V_c| < n$ by König–Egervary theorem. Wlog, by reindexing the vertices if necessary, let $V_c = \{u_1, u_2, \dots, u_s, w_1, w_2, \dots, w_t\}$ be a vertex cover of Γ^c with $|V_c| = s + t < n$.

(Of course, such a vertex cover may consist of only u_i's or only w_j's. That is, $s = 0$ or $t = 0$ is possible.) Let $M = \left[m_{ij}\right]$ be the Γ-PAM s.t. $m_{ij} = 0$ if $u_i \sim w_j$ in Γ. Then,$M = [\{s+1, s+2, \dots, n\} | \{t+1, t+2, \dots, n\}]$, that is, the submatrix of M determined by the rows $s+1, s+2, \dots, n$ and the columns $t+1, t+2, \dots, n$, is the zero matrix $0_{(n-s)x(n-t)}$. (Since V_c is a vertex cover of Γ^c, at least one end-vertex of each edge of Γ^c is in V_c. Therefore, there is no edge $\left\{u_i, w_j\right\}$ with $i \geq s+1$ and $j \geq t+1$ in Γ^c. Therefore, $\left\{u_i, w_j\right\} \in E(\Gamma)$ for each $i \geq s+1$ and $j \geq t+1$.

$\therefore m_{ij} = 0$ if $i \geq s+1$ and $j \geq t+1$.)

Let N be any completion of M. Then, N is singular, that is, $\det(N) = 0$, because $s + t < n$: We can evaluate $\det(N)$ by Laplace expansion wrt the rows $1,2, \dots, s$:

$$\det(N) = \sum (-1)^{sum(\bar{r})+sum(\bar{c})} \det(N\,[\bar{r}|\bar{c}]) \det\,(N(\bar{r}|\bar{c})),$$

where $\bar{r} = (1,2, \dots, s), \bar{c} = (j_1, j_2, \dots, j_s), sum(\bar{r}) = 1 + 2 + \cdots s, sum(\bar{c}) = j_1 + j_2 + \cdots + j_s$, and the summation is taken over all $\bar{c} = (j_1, j_2, \ldots, j_s)$ with $1 \leq j_1 < j_2 < \cdots < j_s$. Then, since $N(\bar{r}|\bar{c})$ is an $(n-s) \times (n-s)$ submatrix of N, and since $n - s > t$, at least one of the column numbers of $N(\bar{r}|\bar{c})$, say j_k is > t. But since $j_k > t$, i.e. $j_k \geq t + 1$, $N(\bar{r}|\bar{c})$ contains a zero column. Therefore, $\det\big(N(\bar{r}|\bar{c})\big) = 0$ for each $\bar{c}$. As a result, every term is zero in the above expansion, and thus $\det(N) = 0$.

$\therefore \Gamma$ is not an NCG. ■

2.2 Chordal Graphs

Chordal graphs are closely related to PDCP, and they appear in a variety of fields of mathematics and have many equivalent definitions.

Definition 2.3 Let Γ be a connected graph. If Γ does not contain any C_k , $k \geq 4$, as an induced subgraph, that is if any C_k, for $k \geq 4$, in Γ has a "chord" (for any cycle C in a graph Ω, an edge $e \in E\,(\Omega) \setminus E(C)$ with end vertices in C is called a "chord" of C), then Γ is called "chordal graph", or is said to be “chordal”.

Example 2.2 For each $n \in \mathbb{N}$, K_n is chordal, because any two vertices are adjacent in K_n. Trees are chordal because a tree does not contain a cycle.

Definition 2.4 Let Γ be a graph with $V(\Gamma) = [n]$. $i \in V(\Gamma)$ is called "simplicial" if $N(i)$ is a clique (i.e., a complete graph) in Γ. A "simplicial elimination ordering" or "perfect elimination ordering (PEO)" of Γ is an ordering of $V(\Gamma) = [n]$, say $j_n, j_{n-1} \dots, j_1$, s.t. j_k is simplicial in $\Gamma_k = \Gamma[S = \{j_1, j_2, \dots, j_k\}]$ for each $k = 1,2, \dots, n$.

Theorem 2.2 (Dirac (1961)) Let Γ be a graph with $V(\Gamma) = [n]$. Then: Γ is chordal iff Γ has PEO.

Proof. (This proof is taken from West (2021).)
($\Leftarrow$) (By contrapositive) Suppose that Γ is not chordal. Then, Γ has a cycle C with no chord. $Let\ \sigma = (j_n, j_{n-1}, \dots, j_1)$ be any ordering of [n], and $let\ j_k$ be the first vertex of C in this ordering. Then, $N(j_k)$ is not a clique, because the two neighbors of j_k say a, b, on the cycle C are not adjacent. ($e = \{a, b\} \notin E\ (\Gamma)$, because C does not have any chord, namely, it is chordless.)
$\therefore$ Γ has no PEO.
($\Rightarrow$) For any chordal graph Ω and any $v \in V\ (\Omega), \Omega - \{\text{v}\}$ is again a chordal graph, because deleting a vertex cannot produce a chordless cycle. Therefore, by using induction, it is enough to show that each chordal graph does have a simplicial vertex. Now, we show more: "If Γ is a chordal graph, and if $\Gamma \neq K_n$, then Γ does have two simplicial vertices, say v and w, s.t. $v \nsim w$ in Γ".
Suppose that Γ is not a complete graph. (If Γ is a complete graph, then there is nothing to prove because any ordering of the vertices of Γ is a PEO.) Then, Γ does have a minimal separating set T. (A "separating set" of a graph Γ is a set $S \subseteq V(\Gamma)$ s.t. $\Gamma \setminus S$ has more than one component. If T is a separating set, but any proper subset of T is not, then T is a "minimal separating set".) Since T is minimal, any two $i, j \in T$ have neighbors in any component X of $\Gamma \setminus T$: Suppose not. Then, there are two vertices $i, j \in T$, and a component X of $\Gamma \setminus T$ s.t. one of i, j, say i, does have a neighbor in X, but the other does not have. But then $\Gamma \setminus (T - \{i\})$ is disconnected, namely, $T - \{i\}$ is also a separating set. This contradicts with the minimality of T.
Now, let $i, j \in T$ and X, Y be two components of $\Gamma \setminus T$. Since i, j both have (the same or different) neighbors in X (respectively, in Y) and since X (respectively, Y) is connected, there is a shortest path, say P_X (respectively, P_Y), passing through X (respectively, Y) between the vertices i and j.

Then, $C = P_X \cup P_Y$ is a cycle in Γ and the length of C is ≥ 4.

$\therefore$ Since Γ is chordal, C must have a chord in Γ. And this chord must be $\{i, j\}$ (that is to say $\{i, j\} \in E\ (\Gamma)$):

First of all, since X and Y are different components of $\Gamma \setminus T$, there is no edge between any two vertices of them. In particular, there is no chord, say $\{x, y\}$, s.t. $x \in X$ and $y \in Y$. Secondly, since P_X (respectively, P_Y) is a shortest $i - j$ path through X (respectively, Y), there is no chord, say $\{u, v\}$, with both $u, v \in X$ (respectively, $u, v \in Y$). The only remaining possibility is that $\{i, j\} \in E(\Gamma)$, and thus it is a chord of C. Since the vertices $i, j \in T$ are randomly chosen, T is a clique.

Now, let $\Gamma_1 = \Gamma\ [T \cup X]$ and $\Gamma_2 = \Gamma[T \cup Y]$. First of all, since Γ_1 and Γ_2 are subgraphs of the chordal graph Γ, both are also chordal. If Γ_1 (respectively, Γ_2) is a complete graph, then any vertex $v \in \Gamma_1 \setminus T$ (respectively, $v \in \Gamma_2 \setminus T$) is simplicial. ($v \in T$ is not simplicial, because v has neighbors in X, say v_X, and in Y, say v_Y, but $v_X \nsim v_Y$ in Γ, because v_X and v_Y are in different components of $\Gamma \setminus T$.) If Γ_1 (respectively, Γ_2) is not a complete graph; then, (since $\Gamma_1 \subseteq \Gamma \setminus Y$ (respectively, $\Gamma_2 \subseteq \Gamma \setminus X$) is a proper subgraph of Γ, $|V(\Gamma_1)| < |V(\Gamma)|$ (respectively, $|V(\Gamma_2)| < |V(\Gamma)|$), and thus,) by the induction assumption, Γ_1 (respectively, Γ_2) has two nonadjacent simplicial vertices. And since T is a clique (that is, any two vertices in T are adjacent), one of these vertices of Γ_1 (respectively, Γ_2), say s_X (respectively, say s_Y) is outside T. Finally, since $s_X \in \Gamma_1 \setminus T$, (respectively, $s_Y \in \Gamma_2 \setminus T$), by definition of Γ_1 (respectively, Γ_2) , $N_\Gamma(s_X) \subseteq \Gamma_1$ (respectively, $N_\Gamma(s_Y) \subseteq \Gamma_2$). Therefore, both s_X and s_Y are simplicity in Γ; and since they lie in different components of $\Gamma \setminus T$, they are also nonadjacent in Γ. ■

Definition 2.5 Let Γ be a graph, and $\Omega \subseteq \Gamma$ be a clique in Γ. If there exists no clique containing Ω properly, then Ω is called a "maximal clique".

Lemma 2.1 Let Γ be chordal and $V(\Gamma) = [n]$. Assume that there is an $f = \{k, l\} \in E(\Gamma)$ s.t. $\Gamma \setminus \{f\}$ is also chordal. Let $N(k, l) = \{j \in V\ (\Gamma) \mid j \sim k \text{ and } j \sim l\}$, and let $S = \{k\} \cup \{l\} \cup N(k, l)$. Then $\Omega = \Gamma[S]$ is a clique, and it is also maximal.

Proof. First, Ω is a clique: We need to show that for any x and y, $x \neq y$, in $V\ (\Omega)$, $x \sim y$. Suppose not. Then there are two distinct $x, y \in V\ (\Omega)$ s.t. $x \nsim y$. But then $k - x - l - y - k$ is a C_4 induced by the set $S = \{k, l, x, y\}$ in $\Gamma \setminus \{f\}$. (Note that $f = \{k, l\} \notin \Gamma \setminus \{f\}$, and by assumption, $x \nsim y$. Therefore, C_4 is an induced cycle, that is, it has no chord.) This contradicts with the hypothesis that $\Gamma \setminus \{f\}$ is chordal.
Second, Ω is maximal: Suppose not. Then, there is a clique Λ in Γ s.t. $\Omega \subseteq \Lambda$ but $\Omega \neq \Lambda$. Thus, there is a vertex $v \in \Lambda \setminus \Omega$. But, since Λ is a clique, v $\sim k$ and $v \sim l$. Therefore, $v \in N(k, l)$. Hence $v \in \Omega$, and this obviously contradicts with the assumption that $v \in \Lambda \setminus \Omega$. As a result, there is no clique containing properly Ω. That is, Ω is maximal. ■

Lemma 2.2 Let $K_n \neq \Gamma$ be chordal and $V(\Gamma) = [n]$. Then there are $k, l \in V(\Gamma)$ s.t. $k \nsim l$, and for $f = \{k, l\}$, $\Omega = \Gamma + f$ is chordal.

Proof. Wlog, by renaming if necessary, suppose that $n, n-1, .., 1$ is a PEO of $V(\Gamma)$. Since $\Gamma \neq K_n$ there is the smallest $k \in V\ (\Gamma) = [n]$ s.t. $\Gamma\ [\{1,2, \dots, k\}]$ is not a clique. By the minimality of k, there is $l < k$ s.t $l \nsim k$. (Since k is minimal, for any $j < k, \Gamma\ [\{1,2, \dots, j\}]$ is a clique. Therefore for $l < k$, $l \sim j$ for any $(l \neq) j < k$.) Let $f = \{k, l\}$, and $\Omega = \Gamma + f$. Then, $n, n-1, \dots, 1$ is also PEO for Ω : For $j \leq k$, $\Lambda = \Omega\ [\{1,2, \dots, \mathrm{j}-1\}]$ is a clique, by the minimality of k; and thus, $N(k) = \Lambda$ is a clique in $\Omega\ [\{1,2, .., \mathrm{j}\}]$. For $j > k$, nothing is changed, because we only add the edge $f = \{k, l\}$ to Γ to obtain Ω; and thus, $N(j)$ in $\Omega[\ \{1,2, .., \mathrm{j}\}]$ and in $\Gamma\ [\{1,2, \dots, j\}]$ are the same. (More precisely, $l < k < j$, and since $k \nsim l$, $k, l \notin N_{\Gamma[\{1,2,\dots,j\}]}(j)$. On the other hand, since $\Omega \setminus \Gamma = f, k, l \notin N_{\Omega[\{1,2,\dots,j\}]}(j)$.)
$\therefore n, n_1, \dots, 1$ is also a PEO for $V(\Omega)$.
$\therefore$ By the previous theorem, Ω is chordal. ■

2.3 Positive Definite Completion (PDC)

Definition 2.6 Let $M = [m_{ij}]$ be an $n \times n$ matrix. If some entries of M are assigned real numbers and the others are unassigned s.t. for $i \neq j$, if m_{ij} is assigned a real number, then m_{ji} is also assigned a real number and $m_{ji} = m_{ij}$; then M is called a "partial symmetric matrix (PSM)". We also suppose that m_{ii} is assigned a real number for all $i = 1,2, \dots, n$. Let $M = [m_{ij}]$ be an $n \times n$ PSM. If for every completely non-empty (that is, each entry is assigned a real number) principal submatrix N of M, $\det(N) > 0$ (respectively, $\det(N) \geq 0$), then M is called a "partial positive definite matrix (PPDM)" (respectively, "partial positive semi-definite matrix (PPSDM)").

Definition 2.7 Let $M = [m_{ij}]$ be PSM. Then, the graph Γ_M with $V(\Gamma_M) = [n]$ and $E(\Gamma_M) = \{\{i, j\} \mid i \neq j$ and m_{ij} (and thus m_{ji}) is assigned a real number$\}$ (that is, for $i \neq j, i \sim j$ if f m_{ij} (and thus m_{ji}) is assigned a real number) is called a "specification graph (SG)" of M. It is also said that "M has SG Γ_M" or that "Γ_M is the SG associated with M".

Definition 2.8 Let Γ be a graph s.t. $V(\Gamma) = [n]$. If every PPDM (respectively, PPSDM) M with the SG Γ is completable to a PDM (respectively, PSDM), then Γ is called "positive definite completable graph (PDCG)" (respectively, "positive semi-definite completable graph (PSDCG)").

Lemma 2. 3 Let Γ be a graph. Then: Γ is PDCG $\Leftrightarrow$ it is PSDCG.

Proof.

($\Leftarrow$) Let M be a PPDM with the SG Γ. Then, $\exists\, \varepsilon > 0$ s.t. $N = M - \varepsilon I$ is a PPSDM. Since the same entries of N and M are assigned real numbers, the SG of N is also Γ. Therefore, since Γ is PSDCG by assumption, N is completable to a PSDM, say $\widetilde{N}$. Then, $\widetilde{M} = \widetilde{N} + \varepsilon I$ is a PDM completion of M.

$\therefore\ \Gamma$ is PDCG.

(Note that $\widetilde{M} = \widetilde{N} + \varepsilon I$ is a PDM:

$\det(xI - \widetilde{\mathrm{M}}) = \det(xI - (\widetilde{N} + \varepsilon I)) = \det((x - \varepsilon)I - \widetilde{N})$.

$\therefore\ \eta$ is an eigenvalue of $\widetilde{N}$ $\Leftrightarrow \det(\eta I - \widetilde{N}) = 0$

$$\Leftrightarrow \det(((\eta + \varepsilon) - \varepsilon)I - \widetilde{N}) = 0$$

$$\Leftrightarrow \det\left((\eta + \varepsilon)I - (\widetilde{N} + \varepsilon I)\right) = 0$$

$$\Leftrightarrow \det((\eta+\varepsilon)\,I-\widetilde{M})=0$$
$$\Leftrightarrow \eta+\varepsilon \text{ is an eigenvalue of } \widetilde{M}.$$

∴ Since $\varepsilon > 0$, and since all the eigenvalues of $\widetilde{N}$ are ≥ 0, all the eigenvalues of $\widetilde{M} > 0$.

∴ $\widetilde{M}$ is a PDM.)

(⇒) Let $M=[m_{ij}]$ be a PPSDM with the SG Γ. For each $j \in \mathbb{Z}^+$, let $N_j = M + \frac{1}{j}\, I$. Then N_j is a PPDM. And again, the SG of N_j is Γ as well. Therefore, since Γ is PDCG by assumption, N_j is completable to a PDM, say $\widetilde{N_J}$. Since the modulus of each off-diagonal entry of a PDM is ≤ the maximum diagonal entry, and since the diagonal entries of $\widetilde{N_J}$ are $\leq \max_{i\in[n]}\{m_{ii}+1\}$, all the entries of $\widetilde{N_J}$ are bounded. Therefore, the sequence (or a subsequence of the sequence) of matrices $\widetilde{N}_1, \widetilde{N}_2, \ldots$ is convergent to a matrix, say $\lim_{j\to\infty} \widetilde{N_J}$ = N (or $\lim_{j_k\to\infty} \widetilde{N}_{j_k} = N$). Then, it can be shown that N is a PSDM completion of M.

∴ Γ is a PSDCG. ■

Lemma 2.4 C_4 is not a PDCG.

Proof. By the previous lemma, it is enough to show that C_4 is not PSDCG.

First of all, let $N=\begin{bmatrix}1&1&z\\1&1&1\\z&1&1\end{bmatrix}$. Then:

$$\det(N)=\begin{vmatrix}1&1&z\\1&1&1\\z&1&1\end{vmatrix} \overset{[-r_1+r_2\to r_2]}{=} \begin{vmatrix}1&1&z\\0&0&1-z\\z&1&1\end{vmatrix} = (-1)^{(2+3)}(1-z)\begin{vmatrix}1&1\\z&1\end{vmatrix}$$

$$=-(1-z)^2.$$

∴ $\det(N) = -(z-1)^2 \leq 0$.

∴ N is a PDM iff $z=1$:

$z \neq 1 \implies \det(N) = -(z-1)^2 < 0 \implies$ (Odd number of eigenvalues of N, and thus,) at least one eigenvalue of N is $< 0 \implies N$ is not a PSDM.

$$z = 1 \Rightarrow N = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \Rightarrow \det(xI - N) = \begin{vmatrix} x-1 & -1 & -1 \\ -1 & x-1 & -1 \\ -1 & -1 & x-1 \end{vmatrix}$$

$$\Rightarrow \det(xI - N) \overset{[-r_2+r_3 \to r_3]}{=} \begin{vmatrix} x-1 & -1 & -1 \\ -1 & x-1 & -1 \\ 0 & -x & x \end{vmatrix} = x \begin{vmatrix} x-1 & -1 & -1 \\ -1 & x-1 & -1 \\ 0 & -1 & 1 \end{vmatrix}$$

$$\Rightarrow \det(xI - N) \overset{\substack{[r_3+r_1 \to r_1] \\ [r_3+r_2 \to r_2]}}{=} x \begin{vmatrix} x-1 & -2 & 0 \\ -1 & x-2 & 0 \\ 0 & -1 & 1 \end{vmatrix} = x\,.(-1)^{3+3} \begin{vmatrix} x-1 & -2 \\ -1 & x-2 \end{vmatrix}$$

$$\Rightarrow \det(xI - N) = x\left((x-1)(x-2) - 2\right) = x\,(x^2 - 3x) = x^2(x-3).$$

$\Rightarrow$ The eigenvalues of N are 0 (with multiplicity 2) and 3.

$\Rightarrow N$ is a PSDM.

Now, for the 4-cycle $C_4: 1-2-3-4-1,$ consider the following PPSDM M with the SG C_4:

$$M = \begin{bmatrix} 1 & 1 & ? & 0 \\ 1 & 1 & 1 & ? \\ ? & 1 & 1 & 1 \\ 0 & ? & 1 & 1 \end{bmatrix}.$$

Now, first, all the diagonal entries (namely, all the 1×1 principal submatrices) of M are $1 \geq 0$. Second, each of the completely specified 2×2 principal submatrices of M is equal to the matrix $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, and its determinant is $0 \geq 0$. And, by the above observation about the matrix N, in order M to be completed a PSDM, the (1,3) and (2,4) (and thus, (3,1) and (4,2)) entries of M must be assigned 1. But in this case, since $m_{14} = 0$, a PSDC is not possible:

$\det(xI - M)$

$$= \begin{vmatrix} x-1 & -1 & -1 & 0 \\ -1 & x-1 & -1 & -1 \\ -1 & -1 & x-1 & -1 \\ 0 & -1 & -1 & x-1 \end{vmatrix} \overset{\substack{[-r_1+r_4 \to r_4] \\ [-r_2+r_3 \to r_3]}}{=} \begin{vmatrix} x-1 & -1 & -1 & 0 \\ -1 & x-1 & -1 & -1 \\ 0 & -x & x & 0 \\ -(x-1) & 0 & 0 & (x-1) \end{vmatrix}$$

$$= x\,(x-1) \begin{vmatrix} x-1 & -1 & -1 & 0 \\ -1 & x-1 & -1 & -1 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{vmatrix}$$

$$\overset{\substack{[c_4+c_1 \to c_1] \\ [c_3+c_2 \to c_2]}}{=} x\,(x-1) \begin{vmatrix} x-1 & -2 & -1 & 0 \\ -2 & x-2 & -1 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix}$$

$$= x\,(x-1)(-1)^{4+4} \begin{vmatrix} x-1 & -2 & -1 \\ -2 & x-2 & -1 \\ 0 & 0 & 1 \end{vmatrix} = x\,(x-1)(-1)^{3+3} \begin{vmatrix} x-1 & -2 \\ -2 & x-2 \end{vmatrix}$$

$$= x\,(x-1)\left((x-1)(x-2) - 4\right) = x\,(x-1)(x^2 - 3x - 2).$$

∴ Since $\Delta = 9 - 4\,(-2).\,1 = 17 > 0, x^2 - 3x - 2$ has two real roots, and since the multiplication of the roots of it is $-2 < 0$, one of the roots of this polynomial is < 0.

∴ M has a negative eigenvalue.

∴ M is not a PSDM.

As a result, C_4 is not a PSDCG. ■

Now, we state and prove two lemmas that are needed to demonstrate the main result of this chapter.

Lemma 2. 5 Let M be a square matrix of order n, and let $k, l \in [n]$ be s.t. $k \neq l$. Then:

$$\det M(k|k)\,\det M(l|l) - \det M\,(k|l)\,\det M(l|l) = (\det M)(\det M(k,l|k,l)).$$

Proof. It is enough to demonstrate the lemma for a regular M, because if M is singular, then the lemma can be proved by using a continuity argument.

∴ Assume that M is regular and let $N = M^{-1}$. Then, by the Jacobi identity, we have:

$$\det N\,[k, l|k, l] = \frac{\det M\,(k, l|k, l)}{\det M}\cdot \qquad (*)$$

Now, since $A^{-1} = \frac{1}{\det(A)}\, adj(A)$, where $adj(A) = \left[(-1)^{i+j} \det\, A(\,i \mid j\,)\right]^T$, for any invertible matrix A; we have:

$$N[k, l|k, l] = \begin{bmatrix} N_{kk} & N_{kl} \\ N_{lk} & N_{u} \end{bmatrix} = \frac{1}{\det M}\begin{bmatrix} adj(M)_{kk} & adj(M)_{kl} \\ adj(M)_{lk} & adj(M)_{ll} \end{bmatrix}$$

$$= \frac{1}{\det M}\begin{bmatrix} (-1)^{k+k}\det M(k|k) & (-1)^{l+k}\det M(l|k) \\ (-1)^{k+l}\det M(k|l) & (-1)^{l+l}\det M(l|l) \end{bmatrix}$$

$$\therefore \det N\,[k, l|k, l] = \det\left(\frac{1}{\det M}\begin{bmatrix} \det M(k|k) & (-1)^{1+k}\det M(l|k) \\ (-1)^{k+l}\det M(k|l) & \det M(l|l) \end{bmatrix}\right)$$

$$= \frac{1}{(\det M)^2}\det M(k|k)\det M(l|l) - \det M(k|l)\det M(l|k).$$

∴ By using the Jacobi identity, we obtain the result:

$$(\det M)(\det M(k, l|k, l)) = \det M(k|k)\det M(l|l) - \det M\,(k|l)\det M(l|l). \blacksquare$$

Lemma 2.6 Let $k, l \in [n]$ be s.t. $k \neq l$, and let $f = \{k, l\} \in E(K_n)$. Then the graph $K_n \setminus \{f\}$ is a PDCG.

Proof. Wlog, suppose that $f = \{1, n\}$. Let $M = \left[m_{ij}\right]$ be an $n \times n$ PPDM with the SG $K_n \setminus \{f\}$, and let m_{1n} be specified as z.

After this specification, we still denote the obtained matrix as M. Now, since $M^T = M$; $M(1|n) = M(n|1)$. Therefore, by the previous lemma, we have:

$$\det M(1|1)\det M(n|n) - (\det M(1|n))^2 = (\det M)(\det M(1,n|1,n)). \quad (*)$$

By expanding the determinant of $M(1|n)$ along the n th row, we get:

$$\det M(1|n) = (-1)^{n+1}\det M(1,n|1,n) + c, \text{ for some } c \in \mathbb{R}.$$

$\big(c = (-1)^{n+2}\, m_{n2}\det M\,(1,n|2,n) + (-1)^{n+3}\, m_{n3}\det(1,n|3,n) + \cdots +$ $(-1)^{n+(n-1)}\ m_{n(n-1)}\ \det M(1,n|\,n-1,n\big).)$

And since M is a PPDM, $\det M\,(1,n|1,n) > 0$ by the definition of a PPDM. Let

$$z_0 = \frac{1}{\det M(1.n|1.n)}(-1)^n c,$$

and let m_{1n} be specified as z_0.

Again, after this specification, we still denote the obtained matrix as M. Then:

$$\det M(1|n) = (-1)^{n+1}\, z_0\ \det M(1,n|1,n) + c$$

$$= (-1)^{n+1}\,(-1)^n\ \frac{c}{\det M(1,n|1,n)}\ \det M(1,n|1,n) + c$$

$$= -c + c = 0.$$

$\therefore$ By $(*)$, we have:

$$\det M = \frac{\det M(1|1)\det M(n|n)}{\det M(1,n|1,n)} > 0,$$

because $\det M(1|1)$, $\det M(n|n)$, and $\det M(1,n|1,n)$ are completely specified principal submatrices of the PPDM M, and thus each of them is > 0.

Finally, for each $j = 1,2,..,n-1$, since M is a PPDM, the $j \times j$ leading principal minor (that is, the minor corresponding to the first j rows and the first j columns) of M is > 0. We just proved that $\det M$ is also > 0. Therefore, all the leading principal minors of M are > 0. And thus, M is a PDM.

As a result, since M is arbitrary, for any PPDM M with the SG $K_n \setminus \{f\}$, there is a PDM completing M.

∴ The graph $K_n \setminus \{f\}$ is a PDCG. ■

The last and the main result of this chapter characterizes PDCGs:

Theorem 2.3 Let Γ be a graph and $V(\Gamma) = [n]$. Then Γ is a PDCG iff Γ is chordal.

Proof.

($\Leftarrow$) First of all, if $\Gamma = K_n$, then Γ is trivially a PDCG; simply because any PPDM M is in fact a PDM (all its entries are specified because any two vertices are adjacent in K_n).

∴ Assume that $\Gamma \neq K_n$. Then, by the last lemma of the previous section, $\exists k, l \in V(\Gamma)$ s.t. $k \nsim l$, and $\Omega = \Gamma + f$, where $f = \{k, l\}$, is also a chordal graph.

And since $\Omega \setminus f = \Gamma$ is chordal, by the next to last lemma of the previous section, for $S = (N(k,l) = \{j \in V\ (\Omega) \mid j{\sim}k \text{ and } j{\sim}l\}) \cup \{k,l\}$, $\Lambda = \Omega\ [S]$ is a maximal clique in Ω.

Now, let $M = [m_{ij}]$ be a PPDM with the SG $\Gamma_M = \Gamma$.

Let $N = [n_{ij}]$ be the principal submatrix of M consists of rows and columns of M corresponding to $V(\Lambda)$. Then, since M is a PPDM, N is also a PPDM. Also since $f = \{k,l\} \notin V(\Gamma)$, $n_{kl} = m_{kl}$ is empty, that is, n_{kl} is not assigned a real number. Therefore, the SG of N is $K_m \setminus \{k,l\}$, where $m = |V(\Lambda)|$. And thus, by the previous lemma, N can be completed to a PDM. Therefore, m_{kl} (and m_{lk}) of the PPDM M can be assigned a real number to obtain a matrix, say M_1, $s.t.$ M_1 is again a PPDM with two fewer unassigned entries wrt M. Also, the SG of M_1 is Ω, and Ω is a chordal graph.

Start from the beginning, that is if $\Omega \neq K_n$, then there are $i, j \in V(\Omega)$ s.t. $i \nsim j$, and $\pi = \Omega + e$, where $e = \{i, j\}$, is also a chordal graph, etc.

Continue this procedure, after a finite number of steps, we get a PDM, say R s.t. R is a completion of M.

$\therefore$ Γ is a PDCG.

($\Rightarrow$) We prove the contrapositive of the statement. Assume that Γ is not a chordal graph. Then, by definition, Γ contains an induced subgraph C_4.

Now, by the second lemma of this section, C_4 is not a PDCG.

$\therefore$ Since non-PDCG C_4 is an induced subgraph of Γ, Γ is also not a PDCG. ■

3. LITERATURE REVIEW

First of all, as it is known, there are lots of good resources about graph theory and matrix theory.

One of the best textbooks written in graph theory is West (2002), and the other more comprehensive graduate combinatorial mathematics textbook is West (2021). In particular, an inclusive textbook for chordal graphs is Golumbic (2004).

For matrix theory, we recommend Piziak and Odell (2007), Zhang (2011), or a more detailed textbook by Horn and Johnson (2012). In particular, one of the good textbooks about positive definite matrices, which was also used in the preparation of the thesis, is Berman and Shaked-Monderer (2021). Bapat (2014) is a perfect book combining these two areas of mathematics.

The main theorem of the thesis, namely, "a graph is positive definite completable if and only if it is chordal", was first proved by Grone *et. al.* (1984).

For a survey about matrix completion problems, Johnson (1990) can be referred to.

Finally, about the topic of the thesis, Smith (2008) can also be consulted.

4. CONCLUSIONS AND RECOMMENDATION

This thesis is a review study, it does not contain any original results. As stated before, the source used in the preparation of the main chapter of the thesis is Bapat (2014). For the first chapter, we used other resources, especially we benefited from Piziak and Odell (2007) and Berman and Shaked-Monderer (2021).

The topic of positive definite completion is one of the fundamental topics not only in graph theory but also in many areas of mathematics. In this thesis, we introduced the basic notions and theorems about matrix theory, nonsingular completion, chordal graphs, and positive definite completion problem in graph theory. Also, we surveyed some of the recent results related to positive definite completion in graph theory.

The purpose of this thesis is to introduce these rich and active research areas at a basic level and to present some of the recent results and developments about positive definite completion in graph theory in a very compact form. In other words, our purpose is not to solve an open problem in these areas or to obtain an original result about these areas. However, we aim to present a survey or a review/tutorial source about matrix theory and positive definite completion in graph theory for non-experts in these areas. In other words, we aim our thesis to be an introduction source related to these areas. Therefore, we hope this self-contained thesis will be useful for students and researchers who want to learn the basics of these immensely enjoyable, fascinating, and influential areas of mathematics.

REFERENCES

Bapat, R.B. 2014. Graphs and Matrices (2nd Ed.). Springer, 204 pages, Berlin.

Berman, A. and Shaked-Monderer, N. 2021. Copositive and Completely Positive Matrices. World Scientific, 564 pages, Singapore.

Dirac, G. A. 1961. On rigid circuit graphs. Abhandlungen aus dem Mathematischen Seminar der Universität Hamburg, 25: 71–76.

Golumbic, M. 2004. Algorithmic Graph Theory and Perfect Graphs (Annals of Discrete Mathematics Volume 57) (2nd Ed.). North Holland, 563 pages, Amsterdam.

Grone, R., Johnson, C.R., Sá, E.M. and Wolkowitz, H. 1984. Positive definite completions of partial hermitian matrices. Linear Algebra Appl. 58: 109–124.

Horn, R. A. and Johnson, C. R. 2012. Matrix analysis (2nd Ed.). Cambridge University Press, 662 pages, Cambridge.

Johnson, C.R. 1990. Matrix completion problems: A survey. Proc. Sympos. Appl. Math., Amer. Math. Soc., Providence 40: 171–198.

Piziak, R. and Odell, P. L. 2007. Matrix theory: From generalized inverses to Jordan form. CRC Press, 548 pages, Boca Rotan.

Smith, R. L. 2008. The positive definite completion problem revisited. Linear Algebra and its Applications 429(7): 1442–1452.

West, D. B. 2002. Introduction to graph theory (2nd Ed.). Prentice-Hall, 588 pages, New Jersey.

West, D. B. 2021. Combinatorial mathematics. Cambridge University Press, 969 pages, Cambridge.

Zhang, F. 2011. Matrix theory: Basic results and techniques (2nd Ed.). Springer, 399 pages, New York.

CURRICULUM VITAE

Personal Information

Name and Surname : Zahraa Ihsan Abdulwahid ALSAUD

Education

MSc	Çankırı Karatekin University Graduate School of Natural and Applied Sciences Department of Mathematics	2022-2024
Undergraduate	University of Karbala Faculty of College Education for Pure Science Department of Mathematics	2009-2012