Bounds on the Extremal Eigenvalues of Positive Definite Matrices

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Bounds on the Extremal Eigenvalues of Positive Definite Matrices

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As the candidate's supervisors, we have approved this thesis for submission.

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Preface

The work described in this dissertation was carried out in the School of Mathematical Sciences, University of KwaZulu-Natal, Durban, from February 2018 to November 2018, under the supervision of Dr P. Singh and co-supervised by Dr V. Singh. This study represents original work by the author and has not otherwise been submitted in any form for any degree or diploma to any other tertiary institution. Where use has been made of the work of others, it is duly acknowledged in the text.

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FACULTY OF SCIENCE AND AGRICULTURE

DECLARATION 1 - PLAGIARISM

I, Thokozani Cyprian Martin Jele, declare that

1. The research reported in this thesis represents my own original research, except where due reference is made.

2. This thesis has not been submitted in the past for any degree at any other institution (academic or otherwise).

3. This thesis does not contain other persons' data, pictures, graphs or other information, unless specifically acknowledged as being sourced from the said persons.

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Abstract

The minimum and maximum eigenvalues of a positive definite matrix are crucial to determining the condition number of linear systems. These can be bounded below and above respectively using the Gershgorin circle theorem. Here we seek upper bounds for the minimum eigenvalue and lower bounds for the maximum eigenvalue. Intervals containing the extremal eigenvalues are obtained for the special case of Toeplitz matrices. The theory of quadratic forms is discussed in detail as it is fundamental in obtaining these bounds.

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Firstly I would like to thank God for keeping me thus far and also thank my family as a whole for all the support they have given me from the day I started my tertiary education till now, many things wouldn't have been possible without my family's support. Baba Jele Nonyanda Luvuno. Mama Magatsheni, ngyaphakamisa ngani. Most importantly I would like to extend my sincere gratitude to my supervisor Dr. Pravin Singh and co-supervisor Dr. Virath Singh for allowing me to do my Master's degree under your supervision, encouraging and pushing me to work hard so I can finish this dissertation in a minimum given period, all the support you have given me throughout the year and making yourselves available anytime I needed help, also for arranging funding for me that covered all my tuition fees and for that I'll be forever grateful.

Not forgetting my friends who we started this tertiary journey together back in 2012, I just want to say to you all thank you for everything ngyabonga bangani bami. Lastly I would like to thank Lerato Mtshali the mother of my son for all the support I've been getting from her since like forever encouraging me to keep pushing everything will be okay at the end, now I can see the light at the end of the tunnel. I'll always appreciate that kind of love. I will forever be grateful to all my support system. Ngiyabonga.

Notations

$\mathbb{C}$	Set of complex numbers
$\mathbb{R}$	Set of real numbers
λ	Eigenvalue
$\mathbf{i}$	$\sqrt{-1}$, complex number
$\mathcal{N}$	Null space
$\|\cdot\|$	Norm
$\|\cdot\|_F$	Frobenius norm
$\sigma(\cdot)$	Spectrum of operator $(\cdot)$
$\rho(\cdot)$	Spectral radius
$M_n(\cdot)$	Matrix of order n
$\perp$	Orthogonal

Contents

Background

Positive definite matrices are the matrix analogues to positive numbers. As a consequence, positive definite matrices are a special class of symmetric matrices. It turns out that many useful matrices fall under this class such as the covariance matrix, overlap matrices used in quantum chemistry and dynamical matrices used in the calculation of molecular vibrations. Quadratic forms on positive definite matrices are useful in optimization problems. Equally important, especially to a mathematician, is the fact that the theorem of definite matrices is an incredibly rich and beautiful field. There are chains of elegant results concerning these matrices, especially for positive definite matrices.

Chapter 1

Introduction

Matrices began in the second century with the Chinese but it was believed that it originated in the 4^{th} century with the Babylonians, even though the first example of matrix methods that were used to solve simultaneous linear equations were written during the Han Dynasty in China [8]. The great progress was then made in the early 18^{th} century in the study of matrices when Carl Gauss (1777-1855) first used the term "determinant" while discussing quadratic forms even though its meaning was not exactly the same as it is known today.

The term "matrices" was first used by James Sylvester (1814-1897) but then his colleague Arthur Cayley (1821-1857) was the first to publish an abstract definition of a matrix in his Memoir on the Theory of Matrices in 1858 [8]. In Linear Algebra, a symmetric matrix is a square matrix that is equal to its transpose, though the essential focus in this dissertation will be on positive definite matrices and the behaviour of their eigenvalues especially the extremal ones.

Eigenvalues can be applied in various fields such as communication systems, designing bridges, designing car stereo system, electrical engineering and mechanical engineering. In communication systems eigenvalues were used by Claude Shannon (1916-2001) to determine the theoretical limit to how much information can be transmitted through a communication medium like your telephone line or through the air [5]. In bridge design, eigenvalues were used to ensure the stability of their construction and in electrical engineering eigenvalues are useful for decoupling three-phase systems through symmetrical component transformation [9].

Positive definite matrices are fundamental objects in applied mathematics, engineering and other mathematical scientific fields. In applied mathematics mostly they appear as Hessian matrices, covariance matrices in statistic and diffusion tensors in medical imaging [12]. Historically, positive definite matrices arise quite naturally in the study of n-ary quadratic forms [5]. Positive definite matrices are employed in certain optimization algorithms in mathematical programming, in testing for the strict convexity of scalar-valued vector functions [5].

A positive definite matrix is a Hermitian matrix with all positive eigenvalues. A class of Hermitian matrices with the special positivity property arises naturally in many applications. The real symmetric matrices with this positivity property is a generalization to matrices of the notion of a positive number [3]. Note that as it is a symmetric matrix all the eigenvalues are real, so it makes sense to talk about them being positive.

Positive definite matrices play an important role when studying general matrices. For any matrix A with complex coefficients, AA^* is positive semidefinite, but $A + A^*$ will have this property only under special circumstances [11]. In other cases the fact that a certain Hermitian matrix associated with A is positive definite gives insight concerning the characteristic roots of A [11]. Charles Hermite (1822-1901) has already studied this idea of characteristics polynomial.

The spectral radius of a square matrix A is defined by $\rho(A) = \max_{\lambda \in \sigma(A)} |\lambda|$. The convergence of iterative schemes for solving linear systems involving A requires that $\rho(A) < 1$. The condition number of matrix A is defined by $\rho(A)\rho(A^{-1})$. For positive definite matrices this is equivalent to $\frac{\lambda_n}{\lambda_1}$ where λ_1 is the smallest eigenvalue and λ_n is the largest.

This dissertation consists of four chapters excluding the introduction and conclusion, and these chapters are organised as follows.

• Chapter 2: In this chapter we study some important properties and theorems relating to Hermitian and symmetric matrices, such as the Rayleigh-Ritz theorem, Courant-Fischer theorem as well as the interlacing property.

• Chapter 3: Here we state and prove some important results pertaining to Positive Definite Matrices

• Chapter 4: We concentrate on finding lower bounds for the maximum eigenvalue of symmetric matrices.

- Chapter 5: Here we concentrate on bounding the extremal eigenvalues of positive definite Toeplitz matrices.

Chapter 2

Hermitian and Symmetric Matrices

Firstly, we give a brief overview of the importance of Hermitian and symmetric matrices.

Example 1. Consider the second-order linear partial differential operator L defined by

$$Lf(\boldsymbol{x}) \equiv \sum_{i,j=1}^{n} a_{ij} \frac{\partial^2 f(\boldsymbol{x})}{\partial x_i x_j}, \tag{2.1}$$

where the coefficients $a_{ij} \in \mathbb{R}$, the function $f(\boldsymbol{x})$ is assumed to be defined on the domain $D \subset \mathbb{R}^n$, and f is twice continuously differentiable on D. The operator L is associated in a natural way with a matrix. The matrix $A = [a_{ij}]$ need not to be symmetric, but since the mixed partial derivative of f are equal, we have from (2.1) that

$$Lf = \sum_{i,j=1}^{n} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j}$$

$$
\begin{aligned}
&= \sum_{i,j=1}^{n} \left[\frac{1}{2} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} + \frac{1}{2} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} \right] \\
&= \sum_{i,j=1}^{n} \frac{1}{2} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} + \sum_{i,j=1}^{n} \frac{1}{2} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} \\
&= \sum_{i,j=1}^{n} \frac{1}{2} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} + \sum_{i,j=1}^{n} \frac{1}{2} a_{ji} \frac{\partial^2 f}{\partial x_j \partial x_i} \\
&= \sum_{i,j=1}^{n} \frac{1}{2} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} + \sum_{i,j=1}^{n} \frac{1}{2} a_{ji} \frac{\partial^2 f}{\partial x_i \partial x_j} \\
&= \sum_{i,j=1}^{n} \frac{1}{2} \big(a_{ij} + a_{ji} \big) \frac{\partial^2 f}{\partial x_i \partial x_j}. \qquad (2.2)
\end{aligned}
$$

Let $\boldsymbol{z}$ be the vector with components $z_i = \frac{\partial}{\partial x_i}$ and $\boldsymbol{y}$ be the vector with components $y_i = \frac{\partial f}{\partial x_i}$.

$$
\begin{aligned}
\boldsymbol{z}^t A \boldsymbol{y} &= \sum_{i,j=1}^{n} z_i a_{ij} y_j \\
&= \sum_{i,j=1}^{n} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} \qquad (2.3) \\
&= Lf.
\end{aligned}
$$

Comparing (2.3) and (2.2) we deduce that L is identified with the matrix A as well as the symmetric matrix $\frac{1}{2}\big(A + A^t\big)$.

Example 2. Let $A = [a_{ij}] \in M_n(\mathbb{C})$ be the complex matrix and consider the sesquilinear form

$$
H(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{y}^* A \boldsymbol{x} = \sum_{i,j=1}^{n} a_{ij} \bar{y}_i x_j \quad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{C}^n.
$$

If $H(\boldsymbol{x}, \boldsymbol{y}) = \overline{H(\boldsymbol{y}, \boldsymbol{x})}$ for all $\boldsymbol{x}, \boldsymbol{y}$, then choose $\boldsymbol{x} = \boldsymbol{e}_j$ and $\boldsymbol{y} = \boldsymbol{e}_i$, to get $H(\boldsymbol{e}_j, \boldsymbol{e}_i) = a_{ij}$

and $H(\boldsymbol{e}_i, \boldsymbol{e}_j) = a_{ji}$. This implies that $a_{ij} = \bar{a}_{ji}$, hence $A = A^*$. Therefore sesquilinear forms are naturally associated with Hermitian matrices.

Theorem 2.1. *Let $A = [a_{ij}] \in M_n(\mathbb{C})$ be Hermitian. Then*

(a) $\boldsymbol{x}^* A \boldsymbol{x}$ is real for all $\boldsymbol{x} \in \mathbb{C}^n$;

(b) All the eigenvalues of A are real,

Proof.

(a)

$$
\begin{aligned}
(\boldsymbol{x}^* A \boldsymbol{x})^* &= \boldsymbol{x}^* A^* \boldsymbol{x}^{**} \\
&= \boldsymbol{x}^* A \boldsymbol{x}.
\end{aligned}
$$

(b) Let $\boldsymbol{x}$ be an eigenvector of A corresponding to eigenvalue λ. Then

$$A\boldsymbol{x} = \lambda \boldsymbol{x} \tag{2.4}$$

$$(A\boldsymbol{x})^* = (\lambda \boldsymbol{x})^*$$

$$\boldsymbol{x}^* A^* = \bar{\lambda} \boldsymbol{x}^*$$

$$\boldsymbol{x}^* A = \bar{\lambda} \boldsymbol{x}^*. \tag{2.5}$$

Postmulitply (2.5) by $\boldsymbol{x}$ to get

$$\boldsymbol{x}^* A \boldsymbol{x} = \bar{\lambda} \boldsymbol{x}^* \boldsymbol{x}. \tag{2.6}$$

And premultiply (2.4) by $\boldsymbol{x}^*$ to get

$$\boldsymbol{x}^* A \boldsymbol{x} = \lambda \boldsymbol{x}^* \boldsymbol{x}. \tag{2.7}$$

Subtracting (2.7) from (2.6) yields

$$(\bar{\lambda} - \lambda)\boldsymbol{x}^*\boldsymbol{x} = \boldsymbol{0}.$$

Hence $\lambda = \bar{\lambda}$ since $\boldsymbol{x} \neq \boldsymbol{0}$ is an eigenvector. □

Theorem 2.2. *If $A \in M_n(\mathbb{R})$ is symmetric then the eigenvectors can be taken as real.*

Proof. Let $\boldsymbol{z} = \boldsymbol{x} + \mathbf{i}\boldsymbol{y}$ be an eigenvector of A corresponding to λ then

$$A\boldsymbol{z} = \lambda\boldsymbol{z},$$

$$A(\boldsymbol{x} + \mathbf{i}\boldsymbol{y}) = \lambda(\boldsymbol{x} + \mathbf{i}\boldsymbol{y}),$$

$$A\boldsymbol{x} + \mathbf{i}A\boldsymbol{y} = \lambda\boldsymbol{x} + \mathbf{i}\lambda\boldsymbol{y}. \tag{2.8}$$

Since λ is real, we can equate real and imaginary parts in (2.8), hence $A\boldsymbol{x} = \lambda\boldsymbol{x}$ and $A\boldsymbol{y} = \lambda\boldsymbol{y}$. Therefore $\boldsymbol{x}$ or $\boldsymbol{y}$ can be taken as eigenvectors which are real. □

Theorem 2.3 (Spectral theorem for Hermitian matrices [6])**.** *Let $A \in M_n(\mathbb{C})$ be given. Then A is Hermitian if and only if there is a unitary matrix $U \in M_n$ and real diagonal matrix $\Lambda \in M_n(\mathbb{C})$ such that $A = U\Lambda U^*$. Moreover, A is real and Hermitian (that is, real symmetric) if and only if there is a real orthogonal matrix $P \in M_n(\mathbb{R})$ and real diagonal matrix $\Lambda \in M_n(\mathbb{R})$ such that $A = P\Lambda P^T$.*

Theorem 2.4 (Rayleigh-Ritz [3])**.** *Let $A \in M_n(\mathbb{C})$ be Hermitian, and let the eigenvalues be ordered as*

$$\lambda_{\min} = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1} \leq \lambda_n = \lambda_{\max},$$

then

$$\lambda_1\boldsymbol{x}^*\boldsymbol{x} \leq \boldsymbol{x}^*A\boldsymbol{x} \leq \lambda_n\boldsymbol{x}^*\boldsymbol{x}. \tag{2.9}$$

For all $\boldsymbol{x} \in \mathbb{C}^n$,

$$\lambda_{\max} = \lambda_n = \max_{\boldsymbol{x} \neq 0} \frac{\boldsymbol{x}^* A \boldsymbol{x}}{\boldsymbol{x}^* \boldsymbol{x}} = \max_{\boldsymbol{x}^* \boldsymbol{x} = 1} \boldsymbol{x}^* A \boldsymbol{x}, \tag{2.10}$$

and

$$\lambda_{\min} = \lambda_1 = \min_{\boldsymbol{x} \neq 0} \frac{\boldsymbol{x}^* A \boldsymbol{x}}{\boldsymbol{x}^* \boldsymbol{x}} = \min_{\boldsymbol{x}^* \boldsymbol{x} = 1} \boldsymbol{x}^* A \boldsymbol{x}. \tag{2.11}$$

Proof. Since A is Hermitian, there exists a unitary matrix $U \in M_n(\mathbb{C})$ that is $UU^* = I$, such that $A = U\Lambda U^*$, where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \cdots, \lambda_n)$. For any $\boldsymbol{x} \in \mathbb{C}^n$, we have

$$\begin{aligned}
\boldsymbol{x}^* A \boldsymbol{x} &= \boldsymbol{x}^* U \Lambda U^* \boldsymbol{x} \\
&= (U^* \boldsymbol{x})^* \Lambda (U^* \boldsymbol{x}) \\
&= \begin{bmatrix} (\overline{U^* \boldsymbol{x}})_1 & , \cdots, & (\overline{U^* \boldsymbol{x}})_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} \begin{bmatrix} (U^* \boldsymbol{x})_1 \\ \vdots \\ (U^* \boldsymbol{x})_n \end{bmatrix} \\
&= \sum_{i=1}^{n} \lambda_i |(U^* \boldsymbol{x})_i|^2 \\
&\leq \lambda_{\max} \sum_{i=1}^{n} |(U^* \boldsymbol{x})_i|^2,
\end{aligned} \tag{2.12}$$

since $\lambda_i \leq \lambda_{\max}$. Similarly

$$\boldsymbol{x}^* A \boldsymbol{x} \geq \lambda_{\min} \sum_{i=1}^{n} |(U^* \boldsymbol{x})_i|^2. \tag{2.13}$$

Also note that

$$\begin{aligned}
\boldsymbol{x}^*\boldsymbol{x} &= (U^*\boldsymbol{x})^*(U^*\boldsymbol{x}) \\
&= \begin{bmatrix} (\overline{U^*\boldsymbol{x}})_1 & , \cdots , & (\overline{U^*\boldsymbol{x}})_n \end{bmatrix} \begin{bmatrix} (U^*\boldsymbol{x})_1 \\ \vdots \\ (U^*\boldsymbol{x})_n \end{bmatrix} \\
&= \sum_{i=1}^{n} |(U^*\boldsymbol{x})_i|^2. \qquad (2.14)
\end{aligned}$$

Using (2.12), (2.13) and (2.14) gives

$$\lambda_{\min}\boldsymbol{x}^*\boldsymbol{x} \leq \boldsymbol{x}^*A\boldsymbol{x} \leq \lambda_{\max}\boldsymbol{x}^*\boldsymbol{x}.$$

Hence, we have shown that

$$\lambda_1\boldsymbol{x}^*\boldsymbol{x} \leq \boldsymbol{x}^*A\boldsymbol{x} \leq \lambda_n\boldsymbol{x}^*\boldsymbol{x}. \qquad (2.15)$$

It then follows from (2.15) that

$$\lambda_1 \leq \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} \leq \lambda_n, \qquad (2.16)$$

for $\boldsymbol{x} \neq \mathbf{0}$.

Equality is attained on the right hand side of (2.16) when $\boldsymbol{x}$ is an eigenvector corresponding to λ_n. Hence, we are justified in writing

$$\max_{\boldsymbol{x}\neq 0} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} = \lambda_n. \qquad (2.17)$$

Since $\boldsymbol{x} \neq \mathbf{0}$, we have

$$\frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} = \left(\frac{\boldsymbol{x}}{\sqrt{\boldsymbol{x}^*\boldsymbol{x}}}\right)^* A \left(\frac{\boldsymbol{x}}{\sqrt{\boldsymbol{x}^*\boldsymbol{x}}}\right)$$

and

$$\left(\frac{\boldsymbol{x}}{\sqrt{\boldsymbol{x}^*\boldsymbol{x}}}\right)^*\left(\frac{\boldsymbol{x}}{\sqrt{\boldsymbol{x}^*\boldsymbol{x}}}\right) = 1.$$

Hence (2.17) is equivalent to the condition

$$\max_{\boldsymbol{x}^*\boldsymbol{x}=1} \boldsymbol{x}^* A \boldsymbol{x} = \lambda_n.$$

A similar argument holds for the right hand side of (2.11). □

Theorem 2.5 (Courant-Fischer [3]). *Let $A \in M_n(\mathbb{C})$ be a Hermitian matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$, and let $1 \leq k \leq n$. Then*

$$\lambda_k = \min_{\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_{n-k}\in\mathbb{C}^n} \max_{\substack{\boldsymbol{x}\neq\boldsymbol{0},\boldsymbol{x}\in\mathbb{C}^n \\ x\perp\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_{n-k}}} \frac{\boldsymbol{x}^* A \boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} \tag{2.18}$$

and

$$\lambda_k = \max_{\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_{k-1}\in\mathbb{C}^n} \min_{\substack{\boldsymbol{x}\neq\boldsymbol{0},\boldsymbol{x}\in\mathbb{C}^n \\ \boldsymbol{x}\perp\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_{k-1}}} \frac{\boldsymbol{x}^* A \boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}}. \tag{2.19}$$

Remark 1. If $k = n$ in (2.18) or $k = 1$ in (2.19) we agree to omit the outer optimization, as the set over which the optimization take place is empty. In these two cases the assertions reduce to the Rayliegh-Ritz theorem.

Proof. Write $A = U\Lambda U^*$ and let $1 \leq k \leq n$. If $\boldsymbol{x} \neq \boldsymbol{0}$

$$\begin{aligned}\frac{\boldsymbol{x}^* A \boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} &= \frac{(U^*\boldsymbol{x})^*\Lambda(U^*\boldsymbol{x})}{\boldsymbol{x}^*\boldsymbol{x}} \\ &= \frac{(U^*\boldsymbol{x})^*\Lambda(U^*\boldsymbol{x})}{(U^*\boldsymbol{x})^*(U^*\boldsymbol{x})}\end{aligned}$$

and $\{U^*\boldsymbol{x} | \boldsymbol{x} \in \mathbb{C}^n \text{ and } \boldsymbol{x} \neq \boldsymbol{0}\} = \{\boldsymbol{y} \in \mathbb{C}^n | \boldsymbol{y} \neq \boldsymbol{0}\}$, where $\boldsymbol{y} = U^*\boldsymbol{x}$. Thus if $\boldsymbol{w}_1, \boldsymbol{w}_2, \cdots, \boldsymbol{w}_{n-k} \in \mathbb{C}^n$ are given, we have

$$\begin{aligned} \sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0} \\ \boldsymbol{x}\perp\boldsymbol{w}_1,\cdots,\boldsymbol{w}_{n-k}}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} &= \sup_{\substack{\boldsymbol{y}\neq\boldsymbol{0} \\ \boldsymbol{y}\perp U^*\boldsymbol{w}_1,\cdots,U^*\boldsymbol{w}_{n-k}}} \frac{\boldsymbol{y}^*\Lambda\boldsymbol{y}}{\boldsymbol{y}^*\boldsymbol{y}} \\ &= \sup_{\substack{\boldsymbol{y}^*\boldsymbol{y}=1 \\ \boldsymbol{y}\perp U^*\boldsymbol{w}_1,\cdots,U^*\boldsymbol{w}_{n-k}}} \boldsymbol{y}^*\Lambda\boldsymbol{y}. \end{aligned} \tag{2.20}$$

Note that

$$\begin{aligned} \boldsymbol{y}^*\Lambda\boldsymbol{y} &= \begin{bmatrix} \bar{y}_1 & ,\cdots, & \bar{y}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \\ &= \sum_{i=1}^{n} \lambda_i |y_i|^2 \end{aligned} \tag{2.21}$$

and

$$\begin{aligned} \boldsymbol{y}^*\boldsymbol{y} &= \begin{bmatrix} \bar{y}_1 & ,\cdots, & \bar{y}_n \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \\ &= \sum_{i=1}^{n} |y_i|^2 = 1. \end{aligned}$$

Therefore from (2.20) and (2.21), we have

$$\begin{aligned} \sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0} \\ \boldsymbol{x}\perp\boldsymbol{w}_1,\cdots,\boldsymbol{w}_{n-k}}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} &= \sup_{\substack{\boldsymbol{y}^*\boldsymbol{y}=1 \\ \boldsymbol{y}\perp U^*\boldsymbol{w}_1,\cdots,U^*\boldsymbol{w}_{n-k}}} \sum_{i=1}^{n} \lambda_i |y_i|^2 \\ &\geq \sup_{\substack{\boldsymbol{y}^*\boldsymbol{y}=1 \\ \boldsymbol{y}\perp U^*\boldsymbol{w}_1,\cdots,U^*\boldsymbol{w}_{n-k} \\ \boldsymbol{y}_1=\boldsymbol{y}_2=\cdots=\boldsymbol{y}_{k-1}=0}} \sum_{i=1}^{n} \lambda_i |y_i|^2 \\ &= \sup_{\substack{|\boldsymbol{y}_k|^2+|\boldsymbol{y}_{k+1}|^2+\cdots+|\boldsymbol{y}_n|^2=1 \\ \boldsymbol{y}\perp U^*\boldsymbol{w}_1,\cdots,U^*\boldsymbol{w}_{n-k}}} \sum_{i=k}^{n} \lambda_i |y_i|^2 \\ &\geq \lambda_k. \end{aligned}$$

This shows that

$$\sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0}\\ \boldsymbol{x}\perp\boldsymbol{w}_1,\cdots,\boldsymbol{w}_{n-k}}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} \geq \lambda_k, \tag{2.22}$$

for any $n-k$ vectors $\boldsymbol{w}_1,\cdots,\boldsymbol{w}_{n-k}$. Let $U = [\boldsymbol{U}_1\ \boldsymbol{U}_2\ \cdots\ \boldsymbol{U}_{n-1}\ \boldsymbol{U}_n]$ be the matrix with columns $\boldsymbol{U}_k,\ k=1,2,\cdots,n$ that diagonalizes A and recall that the columns are eigenvectors of A. Consider the set $\{\boldsymbol{U}_{k+1},\boldsymbol{U}_{k+2},\cdots,\boldsymbol{U}_n\}$.

$$\sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0}\\ \boldsymbol{x}\perp\boldsymbol{U}_{k+1},\boldsymbol{U}_{k+2},\cdots,\boldsymbol{U}_n}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} = \sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0}\\ \boldsymbol{x}\perp\boldsymbol{U}_{k+1},\boldsymbol{U}_{k+2},\cdots,\boldsymbol{U}_n}} \frac{(U^*\boldsymbol{x})^*\Lambda(U^*\boldsymbol{x})}{(U^*\boldsymbol{x})^*(U^*\boldsymbol{x})}. \tag{2.23}$$

Now

$$U^*\boldsymbol{x} = \begin{bmatrix} \boldsymbol{U}_1^* \\ \vdots \\ \boldsymbol{U}_k^* \\ \boldsymbol{U}_{k+1}^* \\ \vdots \\ \boldsymbol{U}_n^* \end{bmatrix} \begin{bmatrix} \boldsymbol{x} \end{bmatrix} = \begin{bmatrix} \boldsymbol{U}_1^*\boldsymbol{x} \\ \vdots \\ \boldsymbol{U}_k^*\boldsymbol{x} \\ \boldsymbol{U}_{k+1}^*\boldsymbol{x} \\ \vdots \\ \boldsymbol{U}_n^*\boldsymbol{x} \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{U}_1^*\boldsymbol{x} \\ \vdots \\ \boldsymbol{U}_k^*\boldsymbol{x} \\ \boldsymbol{0} \end{bmatrix}. \tag{2.24}$$

Using (2.23) and (2.24) we obtain

$$\sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0}\\ \boldsymbol{x}\perp\boldsymbol{U}_{k+1},\boldsymbol{U}_{k+2},\cdots,\boldsymbol{U}_n}} \frac{\sum_{i=1}^{k}\lambda_i|\boldsymbol{U}_i^*\boldsymbol{x}|^2}{\sum_{i=1}^{k}|\boldsymbol{U}_i^*\boldsymbol{x}|^2} \leq \lambda_k\frac{\sum_{i=1}^{k}|\boldsymbol{U}_i^*\boldsymbol{x}|^2}{\sum_{i=1}^{k}|\boldsymbol{U}_i^*\boldsymbol{x}|^2} = \lambda_k.$$

Hence (2.23) becomes

$$\sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0}\\ \boldsymbol{x}\perp\boldsymbol{U}_{k+1},\boldsymbol{U}_{k+2},\cdots,\boldsymbol{U}_n}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} \leq \lambda_k. \tag{2.25}$$

From (2.22) we have

$$\sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0}\\ \boldsymbol{x}\perp\boldsymbol{U}_{k+1},\boldsymbol{U}_{k+2},\cdots,\boldsymbol{U}_n}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} \geq \lambda_k. \tag{2.26}$$

Hence,

$$\sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0}\\ \boldsymbol{x}\perp\boldsymbol{U}_{k+1},\boldsymbol{U}_{k+2},\cdots,\boldsymbol{U}_n}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}} = \lambda_k. \tag{2.27}$$

From (2.22) and (2.27), we conclude that

$$\lambda_k = \inf_{\boldsymbol{w}_1,\ldots,\boldsymbol{w}_{n-k}} \sup_{\substack{\boldsymbol{x}\neq\boldsymbol{0}\\ x\perp\boldsymbol{w}_1,\ldots,\boldsymbol{w}_{n-k}}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}}. \tag{2.28}$$

and we may replace inf and sup with min and max since the extremum is achieved. The argument for (2.19) is similar. □

Theorem 2.6. [3] *Let $A \in M_n(\mathbb{C})$ be a Hermitian matrix, let $\boldsymbol{y} \in \mathbb{C}^n$ be a given vector and $a \in \mathbb{R}$ be a given real number. Let $\hat{A} \in M_{n+1}$ be the Hermitian matrix obtained by adjoining A with $\boldsymbol{y}$ and a as shown below:*

$$\hat{A} \equiv \left[\begin{array}{c:c} A & \boldsymbol{y} \\ \hdashline \boldsymbol{y}^* & a \end{array}\right].$$

Let the eigenvalues of A be denoted by λ_i and the eigenvalues of $\hat{A}$ be denoted by $\hat{\lambda}_i$, and assume that they are arranged in increasing order $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_{n-1} \leq \lambda_n$ and $\hat{\lambda}_1 \leq \hat{\lambda}_2 \leq ... \leq \hat{\lambda}_n \leq \hat{\lambda}_{n+1}$, then

$$\hat{\lambda}_1 \leq \lambda_1 \leq \hat{\lambda}_2 \leq \lambda_2 \leq \hat{\lambda}_3 \leq ... \leq \lambda_{n-1} \leq \hat{\lambda}_n \leq \lambda_n \leq \hat{\lambda}_{n+1}. \tag{2.29}$$

Proof. Let $1 \leq k \leq n$. We want to prove that $\hat{\lambda}_k \leq \lambda_k \leq \hat{\lambda}_{k+1}$. Let $\hat{\boldsymbol{x}} = [\boldsymbol{x}^T \ \ \xi]^T \in \mathbb{C}^{n+1}, \boldsymbol{x} \in \mathbb{C}^n, \xi \in \mathbb{C}$ and $\hat{\boldsymbol{w}}_i = [\boldsymbol{w}_i^T \ \ \omega]^T \in \mathbb{C}^{n+1}, \boldsymbol{w}_i \in \mathbb{C}^n, \omega \in \mathbb{C}$. We then use the result (2.18) from the Courant-Fischer theorem with k replaced $k+1$, n replaced by $n+1$, λ replaced by $\hat{\lambda}$, $\boldsymbol{x}$ replaced by $\hat{\boldsymbol{x}}$ and A replaced by $\hat{A}$, therefore

$$\hat{\lambda}_{k+1} = \min_{\hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2, ..., \hat{\boldsymbol{w}}_{(n+1)-(k+1)} \in C^{n+1}} \ \max_{\substack{\hat{\boldsymbol{x}} \neq \boldsymbol{0}, \hat{\boldsymbol{x}} \in \mathbb{C}^{n+1} \\ \hat{\boldsymbol{x}} \perp \hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2, ..., \hat{\boldsymbol{w}}_{(n+1)-(k+1)}}} \frac{\hat{\boldsymbol{x}}^* \hat{A} \hat{\boldsymbol{x}}}{\hat{\boldsymbol{x}}^* \hat{\boldsymbol{x}}}. \tag{2.30}$$

Let $S_1 = \{\hat{\boldsymbol{x}} \in \mathbb{C}^{n+1} | \hat{\boldsymbol{x}} \perp \hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2, ..., \hat{\boldsymbol{w}}_{n-k}\}$ and

$S_2 = \{\hat{\boldsymbol{x}} \in \mathbb{C}^{n+1} | \hat{\boldsymbol{x}} \perp \hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2, ..., \hat{\boldsymbol{w}}_{n-k}, \boldsymbol{e}_{n+1}\}$ then clearly $S_2 \subseteq S_1$. It now follows that

$$\max_{\substack{\hat{\boldsymbol{x}} \neq \boldsymbol{0} \\ \hat{\boldsymbol{x}} \in S_1}} \frac{\hat{\boldsymbol{x}}^* \hat{A} \hat{\boldsymbol{x}}}{\hat{\boldsymbol{x}}^* \hat{\boldsymbol{x}}} \geq \max_{\substack{\hat{\boldsymbol{x}} \neq \boldsymbol{0} \\ \hat{\boldsymbol{x}} \in S_2}} \frac{\hat{\boldsymbol{x}}^* \hat{A} \hat{\boldsymbol{x}}}{\hat{\boldsymbol{x}}^* \hat{\boldsymbol{x}}} \tag{2.31}$$

From (2.30) and (2.31) it is clear that

$$\hat{\lambda}_{k+1} \geq \min_{\hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2, ..., \hat{\boldsymbol{w}}_{n-k} \in \mathbb{C}^{n+1}} \ \max_{\substack{\hat{\boldsymbol{x}} \neq \boldsymbol{0}, \hat{\boldsymbol{x}} \in \mathbb{C}^{n+1} \\ \hat{\boldsymbol{x}} \perp \hat{\boldsymbol{w}}_1, \hat{\boldsymbol{w}}_2, ..., \hat{\boldsymbol{w}}_{n-k} \\ \hat{\boldsymbol{x}} \perp \boldsymbol{e}_{n+1}}} \frac{\hat{\boldsymbol{x}}^* \hat{A} \hat{\boldsymbol{x}}}{\hat{\boldsymbol{x}}^* \hat{\boldsymbol{x}}} \tag{2.32}$$

Recall that $\hat{\boldsymbol{x}} = [\boldsymbol{x}^T \ \ \xi]^T$, with $\hat{\boldsymbol{x}} \perp \boldsymbol{e}_{n+1}$ implies that $\xi = 0$. Therefore:

$$\hat{\boldsymbol{x}}^*\hat{A}\hat{\boldsymbol{x}} = \begin{bmatrix}\boldsymbol{x}^* & 0\end{bmatrix}\left[\begin{array}{c:c} A & \boldsymbol{y} \\ \hdashline \boldsymbol{y}^* & a \end{array}\right]\begin{bmatrix}\boldsymbol{x} \\ 0\end{bmatrix}$$

$$= \begin{bmatrix}\boldsymbol{x}^* & 0\end{bmatrix}\begin{bmatrix}A\boldsymbol{x} \\ y^*\boldsymbol{x}\end{bmatrix}$$

$$= \boldsymbol{x}^*A\boldsymbol{x}$$

and

$$\hat{\boldsymbol{x}}^*\hat{\boldsymbol{x}} = \begin{bmatrix}\boldsymbol{x}^* & 0\end{bmatrix}\begin{bmatrix}\boldsymbol{x} \\ 0\end{bmatrix}$$

$$= \boldsymbol{x}^*\boldsymbol{x}$$

We also know that $\hat{\boldsymbol{x}} \perp \hat{\boldsymbol{w}}_i$ for $i = 1, 2, ..., n-k$, where $\hat{\boldsymbol{x}} = [\boldsymbol{x}^T\ 0]^T$ and $\hat{\boldsymbol{w}}_i = [\boldsymbol{w}_i^T\ \omega]^T$, which results in $\boldsymbol{x} \perp \boldsymbol{w}_i$, $i = 1, 2, \cdots, n-k$. Inequality (2.32) simplifies to

$$\hat{\lambda}_{k+1} \geq \min_{\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_{n-k}\in\mathbb{C}^n} \max_{\substack{\boldsymbol{x}\neq\boldsymbol{0},\boldsymbol{x}\in\mathbb{C}^n \\ \boldsymbol{x}\perp\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_{n-k}}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}}$$

$$= \lambda_k.$$

For the lower bound on λ_k, we use (2.19) for matrix $\hat{A}$ and apply a similar method used for the upper bound, therefore:

$$\hat{\lambda}_k = \max_{\hat{\boldsymbol{w}}_1,\hat{\boldsymbol{w}}_2,\ldots,\hat{\boldsymbol{w}}_{k-1}\in\mathbb{C}^{n+1}} \min_{\substack{\hat{\boldsymbol{x}}\neq\boldsymbol{0},\hat{\boldsymbol{x}}\in\mathbb{C}^{n+1} \\ \hat{\boldsymbol{x}}\perp\hat{\boldsymbol{w}}_1,\hat{\boldsymbol{w}}_2,\ldots,\hat{\boldsymbol{w}}_{k-1}}} \frac{\hat{\boldsymbol{x}}^*\hat{A}\hat{\boldsymbol{x}}}{\hat{\boldsymbol{x}}^*\hat{\boldsymbol{x}}}$$

$$\leq \max_{\hat{\boldsymbol{w}}_1,\hat{\boldsymbol{w}}_2,\ldots,\hat{\boldsymbol{w}}_{k-1}\in\mathbb{C}^{n+1}} \min_{\substack{\hat{\boldsymbol{x}}\neq\boldsymbol{0} \\ \hat{\boldsymbol{x}}\perp\hat{\boldsymbol{w}}_1,\hat{\boldsymbol{w}}_2,\ldots,\hat{\boldsymbol{w}}_{k-1} \\ \hat{\boldsymbol{x}}\perp\boldsymbol{e}_{n+1}}} \frac{\hat{\boldsymbol{x}}^*A\hat{\boldsymbol{x}}}{\hat{\boldsymbol{x}}^*\hat{\boldsymbol{x}}}$$

$$= \max_{\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_{k-1}\in\mathbb{C}^n} \min_{\substack{\boldsymbol{x}\neq\boldsymbol{0},\boldsymbol{x}\in\mathbb{C}^n \\ \boldsymbol{x}\perp\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_{k-1}}} \frac{\boldsymbol{x}^*A\boldsymbol{x}}{\boldsymbol{x}^*\boldsymbol{x}}$$

$$= \lambda_k.$$

If a given Hermitian matrix is modified by bordering, then the new and old eigenvalues must interlace. □

Definition 2.0.1. Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ be two vectors whose components are arranged in ascending order, that is

$$x_i \leq x_{i+1}, \quad y_i \leq y_{i+1}, \quad i = 1, 2, \cdots, n-1.$$

Then $\boldsymbol{y}$ majorizes $\boldsymbol{x}$ if the following conditions are satisfied

$$\sum_{i=1}^{k} x_i \leq \sum_{i=1}^{k} y_i \qquad k = 1, 2, \cdots, n-1,$$
$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i.$$

Theorem 2.7. *Let $A \in M_n(\mathbb{C})$ be Hermitian. The vector of diagonal entries of A majorizes the vector of eigenvalues of A.*

Proof. Let $\hat{\lambda}_1 \leq \hat{\lambda}_2 \leq \cdots \leq \hat{\lambda}_{n-1} \leq \hat{\lambda}_n$ be the ordered eigenvalues of A. The proof is by induction on the dimension of A. For $n = 1$, $\hat{\lambda}_1 = a_{11}$ and the result holds. Assume the result is true for all dimensions $k \leq n-1$. Let $A_1 \in M_{n-1}(\mathbb{C})$ be the principal submatrix of A obtained by deleting the row and column corresponding to the largest diagonal entry of A. Let $\lambda_1 \leq \cdots \leq \lambda_{n-1}$ be the ordered eigenvalues of A_1. Let $\boldsymbol{x} = [\lambda_i] \in \mathbb{R}^{n-1}$ and rearrange the diagonal entries of A_1 in ascending order and denote elements by $\tilde{a}_{ii}$, that is $\tilde{a}_{11} \leq \tilde{a}_{22} \leq \cdots \leq \tilde{a}_{n-1,n-1}$. Let $\boldsymbol{y} = [\tilde{a}_{ii}] \in \mathbb{R}^{n-1}$. By the induction hypothesis we have $\boldsymbol{y}$ majorizes $\boldsymbol{x}$, that is

$$\sum_{i=1}^{k} \lambda_i \leq \sum_{i=1}^{k} \tilde{a}_{ii}, \qquad k = 1, 2, \cdots, n-1. \tag{2.33}$$

By the interlacing property (2.29) we have

$$\hat{\lambda}_1 \leq \lambda_1 \leq \hat{\lambda}_2 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1} \leq \hat{\lambda}_n,$$

hence

$$\sum_{i=1}^{k} \hat{\lambda}_i \leq \sum_{i=1}^{k} \lambda_i, \quad k = 1, 2, \cdots, n-1. \tag{2.34}$$

From (2.33) and (2.34), we have

$$\sum_{i=1}^{k} \hat{\lambda}_i \leq \sum_{i=1}^{k} \tilde{a}_{ii}, \quad k = 1, 2, \cdots, n-1. \tag{2.35}$$

Also we know that

$$\begin{aligned} \sum_{i=1}^{n} \hat{\lambda}_i &= \sum_{i=1}^{n} a_{ii} \\ &= \text{trace}(A). \end{aligned}$$

□

Chapter 3

Positive Definite Matrices

An $n \times n$ Hermitian matrix A is said to be positive definite if

$$\boldsymbol{x}^* A \boldsymbol{x} > 0 \quad \text{for all nonzero} \quad \boldsymbol{x} \in \mathbb{C}^n. \tag{3.1}$$

If the inequality required in (3.1) is weakened to $\boldsymbol{x}^* A \boldsymbol{x} \geq 0$, then A is said to be positive semidefinite. If A is positive definite, then it is also positive semidefinite.

Lemma 3.1. *If $\boldsymbol{x}^* A \boldsymbol{x} = 0$ for all $\boldsymbol{x} \in \mathbb{C}^n$, then $A = \mathbf{0}$.*

Proof. Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{C}^n$ then

$$(\boldsymbol{x}+\boldsymbol{y})^* A (\boldsymbol{x}+\boldsymbol{y}) = \boldsymbol{x}^* A \boldsymbol{x} + \boldsymbol{y}^* A \boldsymbol{y} + \boldsymbol{x}^* A \boldsymbol{y} + \boldsymbol{y}^* A \boldsymbol{x},$$

$$0 = \boldsymbol{x}^* A \boldsymbol{y} + \boldsymbol{y}^* A \boldsymbol{x}, \tag{3.2}$$

$$(\boldsymbol{x}+\mathbf{i}\boldsymbol{y})^* A (\boldsymbol{x}+\mathbf{i}\boldsymbol{y}) = \boldsymbol{x}^* A \boldsymbol{x} + \boldsymbol{y}^* A \boldsymbol{y} + \mathbf{i}\boldsymbol{x}^* A \boldsymbol{y} - \mathbf{i}\boldsymbol{y}^* A \boldsymbol{x},$$

$$0 = \boldsymbol{x}^* A \boldsymbol{y} - \boldsymbol{y}^* A \boldsymbol{x}. \tag{3.3}$$

From (3.2) and (3.3) it follows that $\boldsymbol{x}^* A \boldsymbol{y} = 0$ for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{C}^n$. Now choose $\boldsymbol{x} = \boldsymbol{e}_i$ and $\boldsymbol{y} = \boldsymbol{e}_j$, then $\boldsymbol{e}_i^* A \boldsymbol{e}_j = a_{ij} = 0$. □

Theorem 3.2. *If* $\boldsymbol{x}^* A\boldsymbol{x} > 0$ *for all* $\boldsymbol{x} \in \mathbb{C}^n$, $\boldsymbol{x} \neq \mathbf{0}$ *then* A *is Hermitian.*

Proof.

$$A = \left(\frac{A + A^*}{2}\right) + \mathbf{i}\left(\frac{A - A^*}{2\mathbf{i}}\right)$$

$$= B + \mathbf{i}C, \tag{3.4}$$

where $B = \frac{A+A^*}{2}$ and $C = \frac{A-A^*}{2\mathbf{i}}$ are Hermitian matrices, then

$$\boldsymbol{x}^* A\boldsymbol{x} = \boldsymbol{x}^* B\boldsymbol{x} + \mathbf{i}\boldsymbol{x}^* C\boldsymbol{x}, \tag{3.5}$$

$$(\boldsymbol{x}^* A\boldsymbol{x})^* = \boldsymbol{x}^* B\boldsymbol{x} - \mathbf{i}\boldsymbol{x}^* C\boldsymbol{x}. \tag{3.6}$$

By subtracting (3.6) from (3.5) we get that $\boldsymbol{x}^* C\boldsymbol{x} = 0$ since the left hand side of (3.5) and (3.6) are equal as both are real numbers. Using Lemma 3.1 we have $C = \mathbf{0}$, which implies that $A = A^*$. Thus a positive definite matrix A may be defined by $\boldsymbol{x}^* A\boldsymbol{x} > 0$ for all $\boldsymbol{x} \in \mathbb{C}^n$, omitting the word Hermitian. □

Example 3. Hessians, minimization, and convexity.

Let $f(\boldsymbol{x})$ be the smooth real-valued function on some domain $D \subset \mathbb{R}^n$. If $\boldsymbol{y} = [y_i]$ is an interior point of D, then Taylor's theorem states that

$$f(\boldsymbol{x}) = f(\boldsymbol{y}) + \sum_{i=1}^{n}(x_i - y_i)\frac{\partial f}{\partial x_i}\bigg|_{\boldsymbol{y}} + \sum_{i,j=1}^{n}(x_i - y_i)(x_j - y_j)\frac{\partial^2 f}{\partial x_i \partial x_j}\bigg|_{\boldsymbol{y}} + \cdots$$

for points $\boldsymbol{x} \in D$ which are near $\boldsymbol{y}$. If $\boldsymbol{y}$ is a critical point of f, then all the first order partial derivatives vanish at $\boldsymbol{y}$ and we have the expression

$$f(\boldsymbol{x}) - f(\boldsymbol{y}) = \sum_{i,j=1}^{n}(x_i - y_i)(x_j - y_j)\frac{\partial^2 f}{\partial x_i \partial x_j}\bigg|_{\boldsymbol{y}} + \cdots$$

$$= (\boldsymbol{x} - \boldsymbol{y})^T H(f; \boldsymbol{y})(\boldsymbol{x} - \boldsymbol{y}) + \cdots$$

for the behavior of f near $\boldsymbol{y}$. The $n \times n$ matrix

$$H(f;\boldsymbol{y}) \equiv \left[\frac{\partial^2 f}{\partial x_i \partial x_j}\Big|_{\boldsymbol{y}} \right]$$

is called the Hessian of f at $\boldsymbol{y}$; it is symmetric because of equality of the mixed partial derivatives of f. Let $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{y}$, then if the quadratic form

$$\boldsymbol{z}^T H(f;\boldsymbol{y})\boldsymbol{z}, \quad \boldsymbol{z} \neq \boldsymbol{0}, \quad \boldsymbol{z} \in \mathbb{R}^n, \tag{3.7}$$

is always positive, then $\boldsymbol{y}$ is the relative minimum for f. If this quadratic form is always negative, then $\boldsymbol{y}$ is a relative maximum for f.

Example 4. Algebraic moments of nonnegative functions.

Let $f(x)$ be an absolute integrable real-valued function on the unit interval $[0,1]$ and consider the numbers

$$a_i = \int_0^1 x^i f(x)dx.$$

The sequence $a_0, a_1, a_2, \cdots$ is said to be a Hausdorff moment sequence, and it is naturally associated with the real quadratic form.

$$\begin{aligned}
\sum_{i,j=0}^{n} a_{i+j} z_i z_j &= \sum_{i,j=0}^{n} \int_0^1 x^{i+j} z_i z_j f(x)dx \\
&= \int_0^1 \left(\sum_{i=0}^{n} x^i z_i\right)\left(\sum_{j=0}^{n} x^j z_j\right) f(x)dx \\
&= \int_0^1 \left(\sum_{i=0}^{n} z_i x^i\right)^2 f(x)dx.
\end{aligned}$$

If we set $A \equiv [a_{ij}] = [a_{i+j}]$, then A will be a symmetric real matrix and we shall have $\boldsymbol{z}^T A \boldsymbol{z} > 0$ for all $\boldsymbol{z} \in \mathbb{R}^{n+1}$ if $f(x) > 0$ for all $x \in [0,1]$. This is true for each $n = 0, 1, 2, \cdots$. A matrix whose elements a_{ij} that are a function only of $i + j$ is called a Hankel matrix.

Example 5. Trigonometric moments of nonnegative functions.

Let $f(\theta)$ be an absolutely integrable real-valued function on $[0, 2\pi]$ and consider the numbers

$$a_i = \int_0^{2\pi} e^{\mathbf{i}i\theta} f(\theta) d\theta, \quad i = 0,\ \pm 1,\ \pm 2, \cdots$$

The sequence a_i is said to be a Toeplitz moment sequence, and it is associated with the quadratic form

$$\sum_{i,j=0}^{n} a_{i-j} z_i \bar{z}_j = \sum_{i,j=0}^{n} \int_0^{2\pi} e^{\mathbf{i}(i-j)\theta} z_i \bar{z}_j f(\theta) d\theta \tag{3.8}$$

$$= \int_0^{2\pi} \left(\sum_{i=0}^{n} e^{\mathbf{i}i\theta} z_i \right) \left(\sum_{j=0}^{n} e^{-(\mathbf{i}j\theta)} \bar{z}_j \right) f(\theta) d\theta$$

$$= \int_0^{2\pi} \left(\sum_{i=0}^{n} e^{\mathbf{i}i\theta} z_i \right) \left(\overline{\sum_{i=0}^{n} e^{\mathbf{i}i\theta} z_i} \right) f(\theta) d\theta \tag{3.9}$$

$$= \int_0^{2\pi} \left| \sum_{i=0}^{n} z_i e^{\mathbf{i}i\theta} \right|^2 f(\theta) d\theta.$$

If we set $A \equiv [a_{ij}] = [a_{i-j}]$, then A will be Hermitian matrix and we shall have $\boldsymbol{z}^* A \boldsymbol{z} > 0$ for all $\boldsymbol{z} \in \mathbb{C}^{n+1}$ if $f(\theta) > 0$ for all $\theta \in [0, 2\pi]$. This is true for each $n = 1, 2, \cdots$. A matrix with elements a_{ij} that are a function only of $i - j$ is called a Toeplitz matrix.

3.1 Properties

Proposition 3.2.1. *Any principal submatrix of a positive definite matrix is positive definite.*

Proof. Let S be a proper subset of $1, 2, \cdots, n$, and denote by $A(S)$ the matrix resulting by extracting rows and columns indicated by S from the positive definite matrix $A \in M_n(\mathbb{C})$. Then $A(S)$ is the principal submatrix of A, and all the principal submatrices arise in this manner, recall that the number $\det(A(S))$ is the principal minor of A. Let $\boldsymbol{x} \in \mathbb{C}^n$ be a nonzero vector with arbitrary entries in the components indicated by S and zero entries elsewhere. Let $\boldsymbol{x}(S)$ denote the vector obtain from $\boldsymbol{x}$ by deleting the zero components from $\boldsymbol{x}$, and observe that

$$\boldsymbol{x}(S)^* A(S) \boldsymbol{x}(S) = \boldsymbol{x}^* A \boldsymbol{x} > 0.$$

Since $\boldsymbol{x}(S) \neq \mathbf{0}$ is arbitrary, this means that $A(S)$ is positive definite. □

Example 6. Consider a 5×5 positive definite matrix and $S = \{1, 3, 4\}$, then

$$A(S) = \begin{bmatrix} a_{11} & a_{13} & a_{14} \\ a_{31} & a_{33} & a_{34} \\ a_{41} & a_{43} & a_{44} \end{bmatrix}.$$

Let $\boldsymbol{x} = [x_1, 0, x_3, x_4, 0]^T$ be arbitrary with x_1, x_3, x_4 not all zero, then vector $\boldsymbol{x}(S) = [x_1, x_3, x_4]^T$, which results in

$$\begin{aligned} \boldsymbol{x}(S)^* A(S) \boldsymbol{x}(S) &= \boldsymbol{x}^* A \boldsymbol{x} \\ &= \sum_{i,j \in S} a_{ij} \bar{x}_i x_j. \end{aligned}$$

Proposition 3.2.2. *If the main diagonal entries of a positive definite matrix are all 1's then all entries of the matrix are bounded by 1 in absolute value.*

Proof. In proposition 3.2.1 choose $S = \{i, j\}$, then

$$A(S) = \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ij}^* & a_{jj} \end{bmatrix}.$$

Then $\det(A(S)) = a_{ii}a_{jj} - |a_{ij}|^2 > 0$, but $a_{ii} = a_{jj} = 1$ which implies $|a_{ij}| < 1$. □

Proposition 3.2.3. *If A is positive definite then so is A^{-1}.*

Proof.

$$\begin{aligned} \boldsymbol{x}^* A^{-1} \boldsymbol{x} &= \boldsymbol{x}^* A^{-1}(AA^{-1})\boldsymbol{x} \\ &= (A^{-1}\boldsymbol{x})^* A(A^{-1}\boldsymbol{x}) \\ &> 0. \end{aligned}$$

Note that A is Hermitian implies that A^{-1} is also Hermitian. □

Proposition 3.2.4. *The sum of any two positive definite matrices of the same size is positive definite. Any positive linear combination of positive definite matrices is positive definite.*

Proof. Let A and B be positive definite and α and β be positive constants then

$$\begin{aligned} \boldsymbol{x}^*(\alpha A + \beta B)\boldsymbol{x} &= \alpha \boldsymbol{x}^* A \boldsymbol{x} + \beta \boldsymbol{x}^* B \boldsymbol{x} \qquad (3.10) \\ &> 0. \end{aligned}$$

□

Proposition 3.2.5. *Each eigenvalue of a positive definite matrix is a positive real number.*

Proof. Let A be positive definite , $\lambda \in \sigma(A)$ and $\boldsymbol{x}$ be an eigenvector of A associated with λ, then

$$\begin{aligned} \boldsymbol{x}^* A\boldsymbol{x} &= \boldsymbol{x}^* \lambda \boldsymbol{x} \\ &= \lambda \boldsymbol{x}^* \boldsymbol{x}. \end{aligned}$$

Therefore,

$$\lambda = \frac{\boldsymbol{x}^* A\boldsymbol{x}}{\boldsymbol{x}^* \boldsymbol{x}}$$

is positive since it is a ratio of two positive numbers. □

Remark 2. Since $\det(A) = \prod_{i=1}^{n} \lambda_i$ and $\text{trace}(A) = \sum_{i=1}^{n} \lambda_i$ it follows that $\det(A)$ and $\text{trace}(A)$ are positive. This also applies to principal submatrices $A(S)$ of A.

Proposition 3.2.6. *If A is Hermitian and has positive eigenvalues then A is positive definite.*

Proof. Since A is Hermitian $A = U\Lambda U^*$, where U is unitary and Λ is a diagonal matrix containing the eigenvalues of A.

$$\begin{aligned} \boldsymbol{x}^* A\boldsymbol{x} &= \boldsymbol{x}^* U\Lambda U^* \boldsymbol{x} \\ &= \sum_{i=1}^{n} \lambda_i |(U^* \boldsymbol{x})_i|^2 \\ &> 0. \end{aligned}$$

□

Proposition 3.2.7. *If A is positive definite then so are powers A^k, where $k = 1, 2, \cdots$*

Proof. Since A is positive definite it is Hermitian and so is A^k. The eigenvalues of A^k are λ^k where λ are the eigenvalues of A which are positive. Hence A^k is positive definite by Proposition 3.2.6. □

Proposition 3.2.8. *Let $A \in M_n(\mathbb{C})$ be Hermitian, then A is positive definite if and only if $det(A(S_i)) > 0$ for $i = 1, 2, \cdots, n$, where $S_i = \{1, 2, \cdots, i\}$. Here $A(S_i)$ denotes the leading principal submatrix of order i.*

Proof. If A is positive definite then every principal submatrix is positive definite according to Proposition 3.2.1. In particular, the leading principal submatrix are positive definite. Then according to remark 2, $\det(A(S_i)) > 0$. We now prove the reverse statement by using induction to show that $A(S_n) = A$ is positive definite. For $i = 1$, $\det(A(S_1)) = a_{11} > 0$ implies that $A(S_1)$ is positive definite. Assume that the statement is true for $i = k$ and denote the eigenvalues of $A(S_k)$ by

$$0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{k-1} \leq \lambda_k. \tag{3.11}$$

Consider $A(S_{k+1})$ and denote its eigenvalues by

$$\hat{\lambda}_1 \leq \hat{\lambda}_2 \leq \cdots \leq \hat{\lambda}_k \leq \hat{\lambda}_{k+1},$$

then by interlacing property (2.29), we have

$$\hat{\lambda}_1 \leq \lambda_1 \leq \hat{\lambda}_2 \leq \lambda_2 \leq \cdots \leq \lambda_{k-1} \leq \hat{\lambda}_k \leq \lambda_k \leq \hat{\lambda}_{k+1}. \tag{3.12}$$

From (3.12) and (3.11) we conclude that $\hat{\lambda}_i$ are positive for $i = 2, 3, \cdots, k+1$. Since $\det(A(S_{k+1})) = \prod_{i=1}^{k+1} \hat{\lambda}_i > 0$, this implies that $\hat{\lambda}_1 > 0$. Since $A(S_{k+1})$ is Hermitian with positive eigenvalues then by Proposition 3.2.6 it is positive definite. □

Proposition 3.2.9. *The diagonal entries of a positive definite matrix A are positive.*

Proof. Choose $\boldsymbol{x} = \boldsymbol{e}_i$ in (3.1) to obtain $a_{ii} > 0$. $\square$

Proposition 3.2.10. *Let $A \in M_n(\mathbb{C})$ be positive definite.*

(a) *If $C \in M_n(\mathbb{C})$, then C^*AC is positive semidefinite.*

(b) *rank(C^*AC) =rank(C).*

(c) *C^*AC is positive definite if and only if C has rank n.*

Proof.

(a) For $\boldsymbol{x} \in \mathbb{C}^n$ we have $\boldsymbol{x}^*(C^*AC)\boldsymbol{x} = (C\boldsymbol{x})^*A(C\boldsymbol{x}) \geq 0$. This is because A is positive definite and $C\boldsymbol{x} = \boldsymbol{0}$ is a possibility.

(b) We show that $\mathcal{N}(C^*AC) = \mathcal{N}(C)$ where $\mathcal{N}$ denotes the null space. If $\boldsymbol{x} \in \mathcal{N}(C)$ then $C\boldsymbol{x} = \boldsymbol{0}$, hence $C^*AC\boldsymbol{x}$, which implies $\boldsymbol{x} \in \mathcal{N}(C^*AC)$. If $\boldsymbol{x} \in \mathcal{N}(C^*AC)$ then $C^*AC\boldsymbol{x} = \boldsymbol{0}$ which implies $\boldsymbol{x}^*C^*AC\boldsymbol{x} = (C\boldsymbol{x})^*A(C\boldsymbol{x}) = \boldsymbol{0}$. But A is positive definite so $C\boldsymbol{x} = \boldsymbol{0}$, hence $\boldsymbol{x} \in \mathcal{N}(C)$. Then rank($C^*AC$) =rank($C$) which follows from the rank-nullity theorem.

(c) If C^*AC is positive definite then $\det(C^*AC) = \det(C^*)\det(A)\det(C) > 0$. Hence $\det(C) \neq 0$ which implies rank(C) $= n$. If rank(C) $= n$ then (C) nonsingular. From (a) C^*AC is positive semidefinite and if $\boldsymbol{x}^*(C^*AC)\boldsymbol{x} = 0$ then $(C\boldsymbol{x})^*A(C\boldsymbol{x}) = 0$ and since A is positive definite this implies that $C\boldsymbol{x} = \boldsymbol{0}$. But C has full rank so $\boldsymbol{x} = \boldsymbol{0}$. Hence $\boldsymbol{x}^*(C^*AC)\boldsymbol{x} > 0$, for all $\boldsymbol{x} \neq \boldsymbol{0}$. $\square$

Example 7. Consider the positive definite matrix

$$A = \begin{bmatrix} 10 & 3 & 4 & 5 & 6 \\ 3 & 12 & 5 & 6 & 7 \\ 4 & 5 & 7 & 7 & 8 \\ 5 & 6 & 7 & 8 & 9 \\ 6 & 7 & 8 & 9 & 18 \end{bmatrix} \tag{3.13}$$

and let A_k denote the leading principal submatrix of order k. The eigenvalues of A_4 interlace the eigenvalues of A according to (2.29) as shown in table 3.1 below. Here $\sigma(A)$ denotes the spectrum of A.

$\sigma(A_4)$		0.41752		4.28190		7.87904		24.42154	
$\sigma(A)$	0.41132		3.40864		6.54087		8.00000		36.63917

Table 3.1: Interlacing of eigenvalues.

Example 8. Let $S = \{1, 3, 4\}$ then

$$A(S) = \begin{bmatrix} 10 & 4 & 5 \\ 4 & 7 & 7 \\ 5 & 7 & 8 \end{bmatrix}.$$

We now show that $A(S)$ is positive definite by definition,

$$\boldsymbol{x}^*A(S)\boldsymbol{x} = \begin{bmatrix} \bar{x}_1 & \bar{x}_2 & \bar{x}_3 \end{bmatrix} \begin{bmatrix} 10 & 4 & 5 \\ 4 & 7 & 7 \\ 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$= \bar{x}_1(10x_1 + 4x_2 + 5x_3) + \bar{x}_2(4x_1 + 7x_2 + 7x_3) + \bar{x}_3(5x_1 + 7x_2 + 8x_3)$$

$$= 10\bar{x}_1x_1 + 4(\bar{x}_1x_2 + \bar{x}_2x_1) + 5(\bar{x}_1x_3 + \bar{x}_3x_1) \tag{3.14}$$

$$+ 7\bar{x}_2x_2 + 7(\bar{x}_2x_3 + \bar{x}_3x_2) + 8\bar{x}_3x_3. \tag{3.15}$$

We complete the square in the quadratic form (3.14) by using Lagrange's method [6] as follows

$$10\left[\bar{x}_1x_1 + \frac{2}{5}(\bar{x}_1x_2 + \bar{x}_2x_1) + \frac{1}{2}(\bar{x}_1x_3 + \bar{x}_3x_1)\right]$$
$$= 10\left(x_1 + \frac{2}{5}x_2 + \frac{1}{2}x_3\right)\left(\bar{x}_1 + \frac{2}{5}\bar{x}_2 + \frac{1}{2}\bar{x}_3\right) - 2(\bar{x}_2x_3 + \bar{x}_3x_2) - \frac{8}{5}\bar{x}_2x_2 - \frac{5}{2}\bar{x}_3x_3. \tag{3.16}$$

Substituting (3.16) into (3.15) results in

$$10\left|x_1 + \frac{2}{5}x_2 + \frac{1}{2}x_3\right|^2 + \frac{27}{5}\bar{x}_2x_2 + 5(\bar{x}_2x_3 + \bar{x}_3x_2) + \frac{11}{2}\bar{x}_3x_3. \tag{3.17}$$

Completing the square in (3.17) gives

$$
\begin{aligned}
&10\left|x_1+\frac{2}{5}x_2+\frac{1}{2}x_3\right|^2+\frac{27}{5}\left[\bar{x}_2x_2+\frac{25}{27}(\bar{x}_2x_3+\bar{x}_3x_2)\right]+\frac{11}{2}\bar{x}_3x_3\\
=&10\left|x_1+\frac{2}{5}x_2+\frac{1}{2}x_3\right|^2+\frac{27}{5}\left(x_2+\frac{25}{27}x_3\right)\left(\bar{x}_2+\frac{25}{27}\bar{x}_3\right)\\
&-\frac{125}{27}\bar{x}_3x_3+\frac{11}{2}\bar{x}_3x_3\\
=&10\left|x_1+\frac{2}{5}x_2+\frac{1}{2}x_3\right|^2+\frac{27}{5}\left|x_2+\frac{25}{27}x_3\right|^2+\frac{47}{54}|x_3|^2\\
&>0 \text{ for all } \boldsymbol{x}\neq\mathbf{0}.
\end{aligned}
$$

Example 9. Proposition 3.2.8 is illustrated in Table 3.2

k	$\det(A(S_k))$
1	10
2	111
3	455
4	344
5	2688

Table 3.2: Leading principal minors.

An adequate way of checking that a Hermitian matrix is not positive definite is to check that any leading principal minor is non positive.

Example 10. Assemble the eigenvalues of A and its diagonal elements in ascending order in vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ respectively such that

$\boldsymbol{x} = [0.41132, 3.40864, 6.54087, 8.00000, 36.63917]^T$ and $\boldsymbol{y} = [7, 8, 10, 12, 18]^T$, then we verify the majorization theorem 2.7 below in Table 3.3.

k	$\sum_{i=1}^{k} x_i$	$\sum_{i=1}^{k} y_i$
1	0.41132	7
2	3.81996	15
3	10.36083	25
4	18.36083	37
5	55	55

Table 3.3: Majorization property.

Chapter 4

Lower Bounds for the Maximum Eigenvalue

The following work is a detailed study of the article by Walker and Mieghem [14].

Consider the $n \times n$ symmetric matrix A and define A_t by,

$$A_t = \sum_{k=0}^{\infty} f_k A^k t^{-k}, \tag{4.1}$$

where f_k are the coefficients of the Maclaurin series for $f(x)$ given by

$$f(x) = \sum_{k=0}^{\infty} f_k x^k. \tag{4.2}$$

This converges for $|x| < R_f$, where $R_f > 0$ is the radius of convergence. If λ is the eigenvalue of A corresponding to eigenvector $\boldsymbol{v}$, then

$$A_t \boldsymbol{v} = \sum_{k=0}^{\infty} f_k A^k t^{-k} \boldsymbol{v}. \tag{4.3}$$

Since λ is the eigenvalue of A, then $A^k\boldsymbol{v} = \lambda^k\boldsymbol{v}$ and

$$\begin{aligned} A_t\boldsymbol{v} &= \sum_{k=0}^{\infty} f_k\lambda^k t^{-k}\boldsymbol{v} \\ &= \sum_{k=0}^{\infty} f_k \left(\frac{\lambda}{t}\right)^k \boldsymbol{v} \\ &= f\left(\frac{\lambda}{t}\right)\boldsymbol{v}, \end{aligned} \tag{4.4}$$

where (4.4) follows from (4.2). Hence the eigenvalues of A_t are $f\left(\frac{\lambda}{t}\right)$. The series converges for all eigenvalues of A provided we choose

$$t > \frac{\tilde{\lambda}}{R_f}, \tag{4.5}$$

where $\tilde{\lambda} = \max_{1\leq j\leq n}|\lambda_j|$. If $f(x)$ is real for x and increasing, then

$$\lambda_{\max}(A_t) = f\left(\frac{\lambda_{\max}(A)}{t}\right). \tag{4.6}$$

Let $\boldsymbol{u} = [1\cdots 1]^T$ and define $N_k = \boldsymbol{u}^T A^k \boldsymbol{u}$ then from equation (2.17) we have

$$\lambda_{\max}(A_t) \geq \frac{\boldsymbol{u}^T A_t \boldsymbol{u}}{\boldsymbol{u}^T\boldsymbol{u}}. \tag{4.7}$$

From (4.7) and (4.1) we get

$$\begin{aligned} \lambda_{\max}(A_t) &\geq \frac{\boldsymbol{u}^T A_t \boldsymbol{u}}{n} \\ &= \frac{1}{n}\sum_{k=0}^{\infty} f_k \boldsymbol{u}^T A^k \boldsymbol{u} t^{-k} \\ &= \frac{1}{n}\sum_{k=0}^{\infty} f_k N_k t^{-k}. \end{aligned} \tag{4.8}$$

From equation (2.17) we also have

$$\begin{aligned} \lambda_{\max}(A^k) &\geq \frac{\boldsymbol{u}^T A^k \boldsymbol{u}}{\boldsymbol{u}^T\boldsymbol{u}} \\ &= \frac{N_k}{n}. \end{aligned} \tag{4.9}$$

It now follows that

$$N_k \leq n\lambda_{\max}(A^k). \tag{4.10}$$

Since $\lambda(A^k) = [\lambda(A)]^k$ it follows that

$$\begin{aligned} \max \lambda(A^k) &= \max\, [\lambda(A)]^k \\ &\leq \max|\lambda(A)|^k \\ &= \tilde{\lambda}^k. \end{aligned} \tag{4.11}$$

Hence,

$$\lambda_{\max}(A^k) \leq \tilde{\lambda}^k. \tag{4.12}$$

We observe from (4.10) and (4.12) that

$$N_k \leq n\tilde{\lambda}^k. \tag{4.13}$$

Hence,

$$\begin{aligned} \sum_{k=0}^{\infty} f_k N_k t^{-k} &\leq n \sum_{k=0}^{\infty} f_k \tilde{\lambda}^k t^{-k} \\ &= n \sum_{k=0}^{\infty} f_k \left(\frac{\tilde{\lambda}}{t}\right)^k. \end{aligned} \tag{4.14}$$

Hence, from (4.2) the series $\sum_{k=0}^{\infty} f_k N_k t^{-k}$ does converges for $t > \frac{\tilde{\lambda}}{R_f}$. Since $f(x)$ is increasing we have that $f^{-1}(x)$ is also increasing as the graph of latter is a reflection about the line $y = x$. Taking the inverse in (4.6) we get

$$\lambda_{\max}(A) = tf^{-1}(\lambda_{\max}(A_t)).$$

Using (4.13) and taking the inverse in inequality (4.8), we then obtain

$$\lambda_{\max}(A) \geq tf^{-1}\left(\frac{1}{n}\sum_{k=0}^{\infty} f_k N_k t^{-k}\right). \tag{4.15}$$

The aim now is to optimize (4.15) over all possible increasing functions f.

Let $h(z)$ be analytic in an interval centred at $z_0 = 0$ and $G(h(z))$ be analytic in a disk centred at $h(0)$, then

$$G(h(z)) = c_0 + \sum_{k=1}^{\infty} c_k z^k. \tag{4.16}$$

Let $h(z) = p$ and differentiate both sides of (4.16) with respect to z successively to obtain

$$\sum_{k=1}^{\infty} c_k k z^{k-1} = G'(p)h'(z), \tag{4.17}$$

$$\sum_{k=2}^{\infty} 2!c_k \binom{k}{2} z^{k-2} = G^{(2)}(p)(h'(z))^2 + G'(p)h^{(2)}(z), \tag{4.18}$$

$$\sum_{k=3}^{\infty} 3!c_k \binom{k}{3} z^{k-3} = G^{(3)}(p)(h'(z))^3 + 3G^{(2)}(p)h^{(2)}(z)h'(z) + G'(p)h^{(3)}(z), \tag{4.19}$$

$$\begin{aligned}\sum_{k=4}^{\infty} 4!c_k \binom{k}{4} z^{k-4} =& G^{(4)}(p)(h'(z))^4 + 6G^{(3)}(p)(h'(z))^2 h^{(2)}(z) + 4G^{(2)}(p)h^{(3)}(z)h'(z) \\ &+ 3G^{(2)}(p)(h^{(2)}(z))^2 + G'(p)h^{(4)}(z).\end{aligned} \tag{4.20}$$

Set $z = 0$ and let $p_0 = h(0)$ in equations (4.17) - (4.20) to obtain

$$c_1 = G'(p_0)h'(0), \tag{4.21}$$

$$2c_2 = G^{(2)}(p_0)(h'(0))^2 + G'(p_0)h^{(2)}(0), \tag{4.22}$$

$$6c_3 = G^{(3)}(p_0)(h'(0))^3 + 3G^{(2)}(p_0)h^{(2)}(0)h'(0) + G'(p_0)h^{(3)}(0), \tag{4.23}$$

$$\begin{aligned} 24c_4 =& G^{(4)}(p_0)(h'(0))^4 + 6G^{(3)}(p_0)(h'(0))^2h^{(2)}(0) + 4G^{(2)}(p_0)h^{(3)}(0)h'(0) \\ &+ 3G^{(2)}(p_0)(h^{(2)}(0))^2 + G'(p_0)h^{(4)}(0). \end{aligned} \tag{4.24}$$

Let $G = f^{-1}$ and

$$h(z) = \frac{1}{n}\sum_{k=0}^{\infty} f_k N_k z^k. \tag{4.25}$$

It follows that

$$f(G(p)) = p. \tag{4.26}$$

By differentiation with respect to p, we obtain

$$G'(p) = [f'(G(p))]^{-1}. \tag{4.27}$$

Successively differentiating (4.27) with respect to p we obtain the following results

$$G^{(2)}(p) = -\frac{f^{(2)}(G(p))}{[f'(G(p))]^3}, \tag{4.28}$$

$$G^{(3)}(p) = 3\frac{[f^{(2)}(G(p))]^2}{[f'(G(p))]^5} - \frac{f^{(3)}(G(p))}{[f'(G(p))]^4}, \tag{4.29}$$

$$G^{(4)}(p) = -15\frac{[f^{(2)}(G(p))]^3}{[f'(G(p))]^7} + 10\frac{f^{(3)}(G(p))f^{(2)}(G(p))}{[f'(G(p))]^6} - \frac{f^{(4)}(G(p))}{[f'(G(p))]^5}. \tag{4.30}$$

Substituting $p = p_0$ in (4.28) - (4.30) gives

$$G^{(2)}(p_0) = -\frac{f^{(2)}(G(p_0))}{[f'(G(p_0))]^3}, \tag{4.31}$$

$$G^{(3)}(p_0) = 3\frac{[f^{(2)}(G(p_0))]^2}{[f'(G(p_0))]^5} - \frac{f^{(3)}(G(p_0))}{[f'(G(p_0))]^4}, \tag{4.32}$$

$$G^{(4)}(p_0) = -15\frac{[f^{(2)}(G(p_0))]^3}{[f'(G(p_0))]^7} + 10\frac{f^{(3)}(G(p_0))f^{(2)}(G(p_0))}{[f'(G(p_0))]^6} - \frac{f^{(4)}(G(p_0))}{[f'(G(p_0))]^5}. \tag{4.33}$$

Observe from (4.2) and (4.25) that

$$\begin{aligned} p_0 &= h(0) \\ &= f_0 \\ &= f(0). \end{aligned} \tag{4.34}$$

Now from (4.16) and (4.34)

$$\begin{aligned} c_0 &= G(p_0) \\ &= f^{-1}f(0) \\ &= 0. \end{aligned}$$

Equation (4.15), (4.16) and (4.25) gives

$$\lambda_{\max}(A) \geq \sum_{k=1}^{\infty} c_k t^{1-k}. \tag{4.35}$$

Note from equation (4.2) that

$$f^{(k)}(0) = k! f_k \tag{4.36}$$

and from (4.25) that

$$h^{(k)}(0) = \frac{k! N_k f_k}{n}. \tag{4.37}$$

It follows from (4.27), (4.34) and (4.36) that

$$G'(p_0) = \frac{1}{f'(f^{-1}(p_0))} = \frac{1}{f'(0)} = \frac{1}{f_1}. \tag{4.38}$$

Set $G(p_0) = 0$ in equation (4.31) - (4.33) to obtain

$$G^{(2)}(p_0) = -\frac{f^{(2)}(0)}{[f'(0)]^3} = -2\frac{f_2}{f_1^3}, \tag{4.39}$$

$$G^{(3)}(p_0) = 3\frac{[f^{(2)}(0)]^2}{[f'(0)]^5} - \frac{f^{(3)}(0)}{[f'(0)]^4} = 6\left(\frac{2f_2^2}{f_1^5} - \frac{f_3}{f_1^4}\right), \tag{4.40}$$

$$G^{(4)}(p_0) = -15\frac{[f^{(2)}(0))]^3}{[f'(0)]^7} + 10\frac{f^{(3)}(0)f^{(2)}(0)}{[f'(0)]^6} - \frac{f^{(4)}(0)}{[f'(0)]^5} = 120\frac{f_2}{f_1}\left(\frac{f_3}{f_1^5} - \frac{f_2^2}{f_1^6}\right) - 24\frac{f_4}{f_1^5}. \tag{4.41}$$

The first few coefficients c_k are obtained as follows. From (4.21), (4.37) and (4.38) it follows that

$$c_1 = \frac{N_1 f_1}{f_1 n} = \frac{N_1}{n}. \tag{4.42}$$

Also from (4.22) , (4.37)and (4.39) we obtain

$$c_2 = \frac{f_2}{f_1}\left(\frac{N_2}{n} - \frac{N_1^2}{n^2}\right) \tag{4.43}$$

and from (4.23), (4.37) and (4.40) we obtain

$$6c_3 = 6\left(2\frac{N_1^3 f_2^2}{f_1^2} - \frac{N_1^3 f_3}{f_1 n^3}\right) - 12\left(\frac{N_1 N_2 f_2^2}{f_1^2 n^2}\right) + 6\frac{N_3 f_3}{f_1 n}, \tag{4.44}$$

which simplifies to

$$c_3 = \frac{f_3}{f_1}\left(\frac{N_3}{n} - \frac{N_1^3}{n^3}\right) + 2\frac{f_2^2}{f_1^2}\left(\frac{N_1^3}{n} - \frac{N_1 N_2}{n^2}\right). \tag{4.45}$$

Now from (4.24), (4.37) and (4.41) we obtain

$$\begin{aligned} 24c_4 =& 24\frac{N_4 f_4}{f_1 n} - 24\frac{N_1^4 f_4}{f_1 n^4} + 120\frac{N_1^4 f_2 f_3}{f_1^2 n^4} - 72\frac{N_1^2 N_2 f_2 f_3}{f_1^2 n^3} - 48\frac{N_1 N_3 f_2 f_3}{f_1^2 n^2} + 144\frac{N_1^2 N_2 f_2^3}{f_1^3 n^3} \\ & - 120\frac{N_1^4 f_2^3}{f_1^3 n^4} - 24\frac{N_2^2 f_2^3}{f_1^3 n^2}, \end{aligned} \tag{4.46}$$

which simplifies to

$$\begin{aligned} c_4 =& \frac{f_4}{f_1}\left(\frac{N_4}{n} - \frac{N_1^4}{n^4}\right) + \frac{f_2 f_3}{f_1^2}\left(5\frac{N_1^4}{n^4} - 3\frac{N_1^2 N_2}{n^3} - 2\frac{N_1 N_3}{n^2}\right) \\ & + \frac{f_2^3}{f_1^3}\left(6\frac{N_1^2 N_2}{n^3} - 5\frac{N_1^4}{n^4} - \frac{N_2^2}{n^2}\right). \end{aligned} \tag{4.47}$$

Let the Taylor series for $f^{-1}(x)$ about f_0 be represented by

$$f^{-1}(x) = \sum_{k=0}^{\infty} a_k (x - f_0)^k, \tag{4.48}$$

which converges for $|x - f_0| < R_{f^{-1}}$. Let $x = \frac{1}{n}\sum_{k=0}^{\infty} f_k N_k t^{-k}$, to get convergence, we require $\left|\frac{1}{n}\sum_{k=1}^{\infty} f_k N_k t^{-k}\right| < R_{f^{-1}}$. Hence, we have

$$\frac{1}{n}\sum_{k=1}^{\infty} f_k N_k t^{-k} < R_{f^{-1}}. \tag{4.49}$$

Now using $N_k \leq n\tilde{\lambda}^k$ from (4.13), an upper bound for the series is obtained as follows

$$\begin{aligned}
\frac{1}{n}\sum_{k=1}^{\infty} f_k N_k t^{-k} &= \frac{1}{n}\sum_{k=0}^{\infty} f_k N_k t^{-k} - f_0 \\
&\leq \sum_{k=0}^{\infty} f_k \left(\frac{\tilde{\lambda}}{t}\right)^k - f_0 \\
&= f\left(\frac{\tilde{\lambda}}{t}\right) - f_0
\end{aligned}$$

Hence forcing this upper bound to be less than $R_{f^{-1}}$ we get $f\left(\frac{\tilde{\lambda}}{t}\right) < f_0 + R_{f^{-1}}$. Taking the inverse, we obtain $\frac{\tilde{\lambda}}{t} < f^{-1}\left(f_0 + R_{f^{-1}}\right)$, which yields

$$t > \frac{\tilde{\lambda}}{f^{-1}(f_0 + R_{f^{-1}})}. \tag{4.50}$$

Combined with the previous bound $t > \frac{\tilde{\lambda}}{R_f}$ from (4.5) we must choose

$$t > \tilde{\lambda} \max\left(\frac{1}{R_f}, \frac{1}{f^{-1}(f_0 + R_{f^{-1}})}\right). \tag{4.51}$$

Since $\tilde{\lambda}$ is unknown we bypass its usage using the following analysis. Given an eigenvector $\boldsymbol{v}$ of A corresponding to eigenvalue λ we have $\lambda\boldsymbol{v} = A\boldsymbol{v}$ from which

$$\begin{aligned}
|\lambda|\|\boldsymbol{v}\|_1 &= \|\lambda\boldsymbol{v}\|_1 \\
&\leq \|A\boldsymbol{v}\|_1 \\
&\leq \|A\|_1\|\boldsymbol{v}\|_1,
\end{aligned}$$

yielding an upper bound for $|\lambda|$ given by

$$\begin{aligned}
|\lambda| &\leq \|A\|_1 \\
&= \max_{1\leq j\leq n} \sum_{i=1}^{n} |a_{ij}|.
\end{aligned}$$

Hence $\tilde{\lambda} \leq \|A\|_1$. It suffices to choose

$$t > \|A\|_1 \max\left(\frac{1}{R_f}, \frac{1}{f^{-1}(f_0 + R_{f^{-1}})}\right). \tag{4.52}$$

Example 11.

(a) Choose $f(x) = x$, hence $f_k = 0$ for all $k \neq 1$, $f_1 = 1$ and $A_t = \frac{A}{t}$. From (4.8) we obtain

$$\lambda_{\max}(A) \geq \frac{N_1}{n}. \tag{4.53}$$

(b) Choose $f(x) = x^3$, hence $f_k = 0$ for all $k \neq 3$, $f_3 = 1$ and $A_t = \frac{A^3}{t^3}$ and $f^{-1}(x) = x^{\frac{1}{3}}$. From (4.15) we obtain

$$\lambda_{\max}(A) \geq \left(\frac{N_3}{n}\right)^{\frac{1}{3}}. \tag{4.54}$$

(c) Choose $f(x) = \frac{1}{1-x} = \sum_{k=0}^{\infty} x^k$, hence $f_k = 1$ for all k and $f^{-1}(x) = 1 - \frac{1}{x}$. The Taylor series of $f^{-1}(x)$ about $f_0 = 1$ has radius of convergence $R_{f^{-1}} = R_f = 1$. From (4.52) choose $t > 2\|A\|_1$. The first three terms from (4.35) using (4.42)-(4.45), yield

$$\lambda_{\max}(A) \geq \frac{N_1}{n} + \frac{1}{t}\left(\frac{N_2}{n} - \frac{N_1^2}{n^2}\right) + 2\left(\frac{N_3}{2n} - \frac{N_1 N_2}{n^2} + \frac{N_1^3}{2n^3}\right)\frac{1}{t^2} + O(t^{-3}), \tag{4.55}$$

also the first four terms from (4.35) yield

$$\begin{aligned}\lambda_{\max}(A) \geq & \frac{N_1}{n} + \frac{1}{t}\left(\frac{N_2}{n} - \frac{N_1^2}{n^2}\right) + 2\left(\frac{N_3}{2n} - \frac{N_1 N_2}{n^2} + \frac{N_1^3}{2n^3}\right)\frac{1}{t^2} \\ & + \frac{1}{t^3}\left[\frac{N_4}{n} - \frac{(2N_1N_3 + N_2^2)}{n^2} + 3\frac{N_1^2 N_2}{n^3} - \frac{N_1^4}{n^4}\right] + O(t^{-4}).\end{aligned} \tag{4.56}$$

Now

$$
\begin{aligned}
N_1^2 &= (\boldsymbol{u}^T A \boldsymbol{u})^2 \\
&= |\boldsymbol{u}^T A \boldsymbol{u}|^2 \\
&\le \|\boldsymbol{u}\|_2^2 \|A\boldsymbol{u}\|_2^2 \\
&= n\boldsymbol{u}^T A^2 \boldsymbol{u} \\
&= nN_2
\end{aligned}
\tag{4.57}
$$

Divide (4.57) by n^2 to obtain

$$
\frac{N_2}{n} - \frac{N_1^2}{n^2} \ge 0. \tag{4.58}
$$

Thus the second term in (4.55) is non negative.

(d) Choose $f(x) = e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$, hence $f_k = \frac{1}{k!}$ for all $k \ge 0$ and $f^{-1}(x) = \ln(x)$. The Taylor series of $f^{-1}(x)$ about $f_0 = 1$ has radius of convergence $R_{f^{-1}} = 1$, and $R_f = \infty$. From (4.52) choose $t > \frac{\|A\|_1}{\ln 2}$. The first three terms from (4.35) yield

$$
\lambda_{\max}(A) \ge \frac{N_1}{n} + \frac{1}{2t}\left(\frac{N_2}{n} - \frac{N_1^2}{n^2}\right) + \frac{1}{6t^2}\left(\frac{N_3}{n} - 3\frac{N_1 N_2}{n^2} + 2\frac{N_1^3}{n^3}\right) + O(t^{-3}), \tag{4.59}
$$

also when using the first four terms from (4.35) yield

$$
\begin{aligned}
\lambda_{\max}(A) \ge & \frac{N_1}{n} + \frac{1}{2t}\left(\frac{N_2}{n} - \frac{N_1^2}{n^2}\right) + \frac{1}{6t^2}\left(\frac{N_3}{n} - 3\frac{N_1 N_2}{n^2} + 2\frac{N_1^3}{n^3}\right) \\
& + \frac{1}{24t^3}\left[\frac{N_4}{n} - \frac{(4N_1N_3 + 3N_2^2)}{n^2} + 12\frac{N_1^2 N_2}{n^3} - 6\frac{N_1^4}{n^4}\right] + O(t^{-4}).
\end{aligned}
\tag{4.60}
$$

Example 12. Consider the 5×5 positive definite matrix defined in (3.13) with the largest eigenvalue $\lambda_{\max}(A) = 36.6392$. The lower bounds for $\lambda_{\max}(A)$ are calculated using example 11 (a) - (d) and represented in table 4.1 below

Equation	t	Lower bound
(4.53)		35.0000
(4.54)		35.9767
(4.55)	$2\|A\|_1$	35.5347
(4.56)	$2\|A\|_1$	35.5379
(4.59)	$\frac{\|A\|_1}{\ln 2}$	35.2982
(4.60)	$\frac{\|A\|_1}{\ln 2}$	35.3022

Table 4.1: Lower bounds for $\lambda_{\max}(A)$.

It is observed that all bounds are sharper than the classical bound from (4.53).

When A is positive definite we have the following key results:

Lemma 4.1. *It holds that* $N_k \geq \frac{N_1^k}{n^{k-1}}$ *for all* $k = 1, 2, \cdots$

Proof. It is known that we can write

$$\begin{aligned} A^k &= U \Lambda^k U^T \\ &= \sum_{j=1}^{n} \lambda_j^k \boldsymbol{v}_j \boldsymbol{v}_j^T, \end{aligned} \tag{4.61}$$

where U is an orthogonal matrix (that diagonalizes A) with column eigenvectors $\{\boldsymbol{v}_j\}$, and Λ is a diagonal matrix whose entries are the eigenvalues $\{\lambda_j\}$, then

$$\begin{aligned} N_k &= \boldsymbol{u}^T A^k \boldsymbol{u} \\ &= \sum_{j=1}^{n} \boldsymbol{u}^T \lambda_j^k \boldsymbol{v}_j \boldsymbol{v}_j^T \boldsymbol{u} \\ &= \sum_{j=1}^{n} \left(\boldsymbol{u}^T \boldsymbol{v}_j\right)^2 \lambda_j^k. \end{aligned} \tag{4.62}$$

Since $\{\boldsymbol{v}_j\}$ forms a basis for $\mathbb{R}^n$, we can write

$$\boldsymbol{u} = \sum_{j=1}^{n} (\boldsymbol{u}^T \boldsymbol{v}_j) \boldsymbol{v}_j, \tag{4.63}$$

hence

$$\begin{aligned} \boldsymbol{u}^T \boldsymbol{u} &= \sum_{j=1}^{n} \boldsymbol{u}^T (\boldsymbol{u}^T \boldsymbol{v}_j) \boldsymbol{v}_j \\ &= \sum_{j=1}^{n} \left(\boldsymbol{u}^T \boldsymbol{v}_j\right)^2. \end{aligned}$$

Then we have that

$$n = \sum_{j=1}^{n} \left(\boldsymbol{u}^T \boldsymbol{v}_j\right)^2. \tag{4.64}$$

Let a real-valued function g be convex on the interval $[a, b]$, with $x_1, x_2, \cdots, x_n \in [a, b]$ and $\omega_1, \omega_2, \cdots, \omega_n \geq 0$ then we have by Jensen's inequality[10]

$$\frac{\omega_1 g(x_1) + \omega_2 g(x_2) + \cdots + \omega_n g(x_n)}{\omega_1 + \omega_2 + \cdots + \omega_n} \geq g\left(\frac{\omega_1 x_1 + \omega_2 x_2 + \cdots + \omega_n x_n}{\omega_1 + \omega_2 + \cdots + \omega_n}\right). \tag{4.65}$$

Let $g(x) = x^k$ which for $x > 0$ is a convex function. Choose $\omega_j = (\boldsymbol{u}^T \boldsymbol{v}_j)^2$ and $x_j = \lambda_j \geq 0$. Now using (4.63)

$$\begin{aligned} N_1 &= \boldsymbol{u}^T A \boldsymbol{u} \\ &= \sum_{j=1}^{n} \boldsymbol{u}^T (\boldsymbol{u}^T \boldsymbol{v}_j) A \boldsymbol{v}_j \\ &= \sum_{j=1}^{n} (\boldsymbol{u}^T \boldsymbol{v}_j)^2 \lambda_j. \end{aligned} \tag{4.66}$$

Similarly

$$N_k = \sum_{j=1}^{n} \left(\boldsymbol{u}^T \boldsymbol{v}_j\right)^2 \lambda_j^k. \tag{4.67}$$

Using Jensen's inequality we get

$$\begin{aligned}
\frac{N_k}{n} &= \frac{\sum_{j=1}^{n} (\boldsymbol{u}^T \boldsymbol{v}_j)^2 \lambda_j^k}{n} \\
&\geq g\left(\frac{\sum_{j=1}^{n} (\boldsymbol{u}^T \boldsymbol{v}_j)^2 \lambda_j}{n}\right) \\
&= \frac{\left(\sum_{j=1}^{n} (\boldsymbol{u}^T \boldsymbol{v}_j)^2 \lambda_j\right)^k}{n^k} \\
&= \frac{N_1^k}{n^k}.
\end{aligned} \tag{4.68}$$

Therefore $N_k \geq \frac{N_1^k}{n^{k-1}}$. □

Applying (4.68) in (4.8) shows that

$$\begin{aligned}
\lambda_{\max}(A_t) &\geq \frac{1}{n} \sum_{k=0}^{\infty} f_k N_k t^{-k} \\
&\geq \sum_{k=0}^{\infty} f_k \frac{N_1^k}{n^k} t^{-k} \\
&= f\left(\frac{N_1}{tn}\right).
\end{aligned} \tag{4.69}$$

Hence, from inequality (4.15) $\lambda_{\max}(A)$ is bounded below by

$$\begin{aligned}
\lambda_{\max}(A) &\geq t f^{-1}\left(\frac{1}{n} \sum_{k=0}^{\infty} f_k N_k t^{-k}\right) \\
&\geq t f^{-1}\left(f\left(\frac{N_1}{tn}\right)\right) \\
&= \frac{N_1}{n}.
\end{aligned} \tag{4.70}$$

We conclude that if A is positive definite and $f(x)$ is increasing then (4.15) is at least as sharp as the classical bound $\frac{N_1}{n}$. In this case, it follows from (4.68) that the first terms in equations (4.43), (4.45) and (4.47) are positive provided $\frac{f_k}{f_1}$ are positive.

Chapter 5

Bounds on the Extreme Eigenvalues of Positive Definite Toeplitz Matrices.

The following work is a detailed study of the article by Dembo [2].

Let A be a $n \times n$ positive semidefinite matrix that is $\boldsymbol{x}^* A \boldsymbol{x} \geq 0$ for any complex vector $\boldsymbol{x} \in \mathbb{C}^n$. We partition A into blocks as follows

$$A = \left[\begin{array}{c|c} c & \boldsymbol{b}^* \\ \hline \boldsymbol{b} & Q, \end{array}\right] \tag{5.1}$$

where Q is a $(n-1) \times (n-1)$ positive semidefinite matrix, $c \geq 0$ is a scalar, and $\boldsymbol{b} \in \mathbb{C}^{n-1}$. Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be the n eigenvalues of A.

Lemma 5.1. *Let B and C be Hermitian matrices such that $C - B$ is positive semidefinite, that is $B \leq C$ then $\lambda_{\max}(B) \leq \lambda_{\max}(C)$ and $\lambda_{\min}(B) \leq \lambda_{\min}(C)$.*

Proof. Let $\boldsymbol{x} \in \mathbb{C}^n$ such that $\boldsymbol{x}^*\boldsymbol{x} = 1$, then $\boldsymbol{x}^*B\boldsymbol{x} \leq \boldsymbol{x}^*C\boldsymbol{x}$. Hence, $\min_{\boldsymbol{x}^*\boldsymbol{x}=1} \boldsymbol{x}^*B\boldsymbol{x} \leq \min_{\boldsymbol{x}^*\boldsymbol{x}=1} \boldsymbol{x}^*C\boldsymbol{x}$ and $\max_{\boldsymbol{x}^*\boldsymbol{x}=1} \boldsymbol{x}^*B\boldsymbol{x} \leq \max_{\boldsymbol{x}^*\boldsymbol{x}=1} \boldsymbol{x}^*C\boldsymbol{x}$ from which it follows that

$$\lambda_{\min}(B) \leq \lambda_{\min}(C) \tag{5.2}$$

and

$$\lambda_{\max}(B) \leq \lambda_{\max}(C), \tag{5.3}$$

where we have used equation (2.9). □

Lemma 5.2. *Define*

$$\tilde{A}(\eta) = \left[\begin{array}{c|c} c & \boldsymbol{b}^* \\ \hline \boldsymbol{b} & \eta I_{n-1} \end{array}\right], \tag{5.4}$$

where $\eta \geq 0$, then the extremal eigenvalues of $\tilde{A}(\eta)$ are given by

$$\frac{c+\eta}{2} \pm \sqrt{\left(\frac{c-\eta}{2}\right)^2 + \boldsymbol{b}^*\boldsymbol{b}}. \tag{5.5}$$

Proof.

$$\tilde{A}(\eta) - \lambda I_n = \left[\begin{array}{c|c} c-\lambda & \boldsymbol{b}^* \\ \hline \boldsymbol{b} & (\eta-\lambda) I_{n-1} \end{array}\right] \tag{5.6}$$

Let

$$d_n = \det(\tilde{A}(\eta) - \lambda I_n)$$

$$= \begin{vmatrix} c-\lambda & b_1^* & b_2^* & \cdots & b_{n-1}^* \\ b_1 & \eta-\lambda & 0 & \cdots & 0 \\ b_2 & 0 & \eta-\lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{n-1} & 0 & 0 & \cdots & \eta-\lambda \end{vmatrix}.$$

Expanding along the last column to evaluate the determinant gives

$$\begin{aligned} d_n &= (\eta-\lambda)d_{n-1} + (-1)^{1+n}b_{n-1}^*(-1)^{1+n-1}b_{n-1}(\eta-\lambda)^{n-2} \\ &= (\eta-\lambda)d_{n-1} - b_{n-1}^*b_{n-1}(\eta-\lambda)^{n-2} \\ &= (\eta-\lambda)\left[(\eta-\lambda)d_{n-2} - b_{n-2}^*b_{n-2}(\eta-\lambda)^{n-3}\right] - b_{n-1}^*b_{n-1}(\eta-\lambda)^{n-2} \\ &= (\eta-\lambda)^2 d_{n-2} - (\eta-\lambda)^{n-2}\left[b_{n-2}^*b_{n-2} + b_{n-1}^*b_{n-1}\right] \\ &= (\eta-\lambda)^{n-2}d_2 - (\eta-\lambda)^{n-2}\left[b_2^*b_2 + b_3^*b_3 + \cdots + b_{n-1}^*b_{n-1}\right] \\ &= (\eta-\lambda)^{n-2}\left[(c-\lambda)(\eta-\lambda) - b_1^*b_1\right] - (\eta-\lambda)^{n-2}\left[b_2^*b_2 + b_3^*b_3 + \cdots + b_{n-1}^*b_{n-1}\right] \\ &= (\eta-\lambda)^{n-2}\left[(c-\lambda)(\eta-\lambda) - \boldsymbol{b}^*\boldsymbol{b}\right]. \end{aligned} \tag{5.7}$$

Hence, the eigenvalues of $\tilde{A}(\eta)$ are $\lambda = \eta$ of multiplicity $n-2$ and the zeros of the quadratic polynomial $(c-\lambda)(\eta-\lambda) - \boldsymbol{b}^*\boldsymbol{b}$ given by (5.5). □

Theorem 5.3. *Bounds on λ_1 and λ_n are given by*

$$\begin{aligned} \frac{c+\eta_1}{2} + \sqrt{\frac{(c-\eta_1)^2}{4} + \boldsymbol{b}^*\boldsymbol{b}} &\le \lambda_n \\ &\le \frac{c+\eta_{n-1}}{2} + \sqrt{\frac{(c-\eta_{n-1})^2}{4} + \boldsymbol{b}^*\boldsymbol{b}} \end{aligned} \tag{5.8}$$

and

$$\frac{c+\eta_1}{2} - \sqrt{\frac{(c-\eta_1)^2}{4} + \boldsymbol{b}^*\boldsymbol{b}} \leq \lambda_1$$
$$\leq \frac{c+\eta_{n-1}}{2} - \sqrt{\frac{(c-\eta_{n-1})^2}{4} + \boldsymbol{b}^*\boldsymbol{b}}, \tag{5.9}$$

where η_1 *is any lower bound on the minimal eigenvalue of* Q *and* η_{n-1} *is any upper bound on the maximal eigenvalue of* Q*.*

Proof. Note that

$$\tilde{A}(\eta_{n-1}) - A = \left[\begin{array}{c|c} 0 & \mathbf{0} \\ \hline \mathbf{0} & \eta_{n-1}I_{n-1} - Q \end{array}\right] \tag{5.10}$$

is a positive semidefinite matrix, hence $A \leq \tilde{A}(\eta_{n-1})$. Also note that

$$A - \tilde{A}(\eta_1) = \left[\begin{array}{c|c} 0 & \mathbf{0} \\ \hline \mathbf{0} & Q - \eta_1 I_{n-1} \end{array}\right]$$

is also positive semi-definite, hence $\tilde{A}(\eta_1) \leq A$. Thus $\tilde{A}(\eta_1) \leq A \leq \tilde{A}(\eta_{n-1})$. Applying Lemma 5.1, we have $\lambda_{\max}(\tilde{A}(\eta_1)) \leq \lambda_{\max}(A) \leq \lambda_{\max}(\tilde{A}(\eta_{n-1}))$ from which (5.8) follows and $\lambda_{\min}(\tilde{A}(\eta_1)) \leq \lambda_{\min}(A) \leq \lambda_{\min}(\tilde{A}(\eta_{n-1}))$ from which (5.9) follows. □

Theorem 5.4. *Let* A *be a* $n \times n$ *matrix, then*

$$\frac{1}{\sqrt{n}}\|A\|_F \leq \lambda_n \leq \|A\|_F, \tag{5.11}$$

where $\|A\|_F^2 = \sum_{i,j=1}^{n}|a_{ij}|^2$.

Proof.

$$\begin{aligned}\lambda_n^2 &\le \lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 \\ &= \text{trace}(A^2) \\ &= \|A\|_F^2,\end{aligned}$$

from which the right hand side of (5.11) follows. Since

$$\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 \le n\lambda_n^2, \tag{5.12}$$

we get

$$\|A\|_F^2 \le n\lambda_n^2, \tag{5.13}$$

from which the left hand side of (5.11) follows. □

We note that

$$\|A\|_F^2 = \|Q\|_F^2 + 2\boldsymbol{b}^*\boldsymbol{b} + c^2. \tag{5.14}$$

Hence

$$\lambda_n \le \sqrt{\|Q\|_F^2 + 2\boldsymbol{b}^*\boldsymbol{b} + c^2}. \tag{5.15}$$

Now if $\|Q\|_F = \eta_{n-1}$ then we get

$$\lambda_n \le \sqrt{\eta_{n-1}^2 + 2\boldsymbol{b}^*\boldsymbol{b} + c^2}. \tag{5.16}$$

Proposition 5.4.1. *The bound on the right hand side of* (5.8) *is tighter then the bound in* (5.16)*.*

Proof By Contradiction.

Assume that

$$\sqrt{\eta_{n-1}^2 + 2\boldsymbol{b}^*\boldsymbol{b} + c^2} < \frac{c + \eta_{n-1}}{2} + \sqrt{\frac{(c - \eta_{n-1})^2}{4} + \boldsymbol{b}^*\boldsymbol{b}}. \tag{5.17}$$

Then we obtain by algebraic manipulation the following results

$$\begin{aligned}
\sqrt{4\eta_{n-1}^2 + 8\boldsymbol{b}^*\boldsymbol{b} + 4c^2} <& c + \eta_{n-1} + \sqrt{(c - \eta_{n-1})^2 + 4\boldsymbol{b}^*\boldsymbol{b}}, \\
4\eta_{n-1}^2 + 8\boldsymbol{b}^*\boldsymbol{b} + 4c^2 <& (c + \eta_{n-1})^2 + (c - \eta_{n-1})^2 + 4\boldsymbol{b}^*\boldsymbol{b} \\
&+ 2(\eta_{n-1} + c)\sqrt{(c - \eta_{n-1})^2 + 4\boldsymbol{b}^*\boldsymbol{b}}, \\
4\eta_{n-1}^2 + 8\boldsymbol{b}^*\boldsymbol{b} + 4c^2 <& 2\eta_{n-1}^2 + 2c^2 + 4\boldsymbol{b}^*\boldsymbol{b} \\
&+ 2(\eta_{n-1} + c)\sqrt{(c - \eta_{n-1})^2 + 4\boldsymbol{b}^*\boldsymbol{b}}, \\
\eta_{n-1}^2 + 2\boldsymbol{b}^*\boldsymbol{b} + c^2 <& (\eta_{n-1} + c)\sqrt{(c - \eta_{n-1})^2 + 4\boldsymbol{b}^*\boldsymbol{b}}, \\
(\eta_{n-1}^2 + c^2 + 2\boldsymbol{b}^*\boldsymbol{b})^2 <& (\eta_{n-1} + c)^2[(c - \eta_{n-1})^2 + 4\boldsymbol{b}^*\boldsymbol{b}], \\
\eta_{n-1}^4 + c^4 + 2\eta_{n-1}^2 c^2 + 4(\boldsymbol{b}^*\boldsymbol{b})^2 + 4\boldsymbol{b}^*\boldsymbol{b}(\eta_{n-1}^2 + c^2) <& c^4 + \eta_{n-1}^4 - 2\eta_{n-1}^2 c^2 \\
&+ 4\boldsymbol{b}^*\boldsymbol{b}(\eta_{n-1}^2 + c^2) + 8\eta_{n-1} c\boldsymbol{b}^*\boldsymbol{b}, \\
4\eta_{n-1}^2 c^2 - 8\eta_{n-1} c\boldsymbol{b}^*\boldsymbol{b} + 4(\boldsymbol{b}^*\boldsymbol{b})^2 <& 0, \\
(\eta_{n-1} c - \boldsymbol{b}^*\boldsymbol{b})^2 <& 0,
\end{aligned}$$

which is a contradiction. □

Proposition 5.4.2. *Let A be an $n \times n$ circulant matrix, then A is also Toeplitz. In addition suppose that A is positive definite, then the lower bound in* (5.8) *with $\eta_1 = 0$ is tighter than that of* (5.11)*.*

Proof By Contradiction.

Assume that

$$\frac{c}{2} + \sqrt{\frac{c^2}{4} + \boldsymbol{b}^*\boldsymbol{b}} < \frac{1}{\sqrt{n}}\|A\|_F \tag{5.18}$$

$$= \frac{1}{\sqrt{n}}\sqrt{n(c^2 + \boldsymbol{b}^*\boldsymbol{b})}$$

$$= \sqrt{c^2 + \boldsymbol{b}^*\boldsymbol{b}}. \tag{5.19}$$

Then by algebraic manipulation, we obtain

$$c + \sqrt{c^2 + 4\boldsymbol{b}^*\boldsymbol{b}} < \sqrt{4c^2 + 4\boldsymbol{b}^*\boldsymbol{b}}$$

$$2c^2 + 2c\sqrt{c^2 + 4\boldsymbol{b}^*\boldsymbol{b}} + 4\boldsymbol{b}^*\boldsymbol{b} < 4c^2 + 4\boldsymbol{b}^*\boldsymbol{b}$$

$$c^2 + c\sqrt{c^2 + 4\boldsymbol{b}^*\boldsymbol{b}} < 0. \tag{5.20}$$

Which is impossible since c is positive. □

Example 13. Consider the positive definite Toeplitz matrix A defined by

$$A = \begin{bmatrix} 10 & 1 & 2 & 1 \\ 1 & 10 & 1 & 2 \\ 2 & 1 & 10 & 1 \\ 1 & 2 & 1 & 10 \end{bmatrix} \tag{5.21}$$

The extremal eigenvalues are given by $\lambda_1 = 8.0000$ and $\lambda_4 = 14.0000$.

The various upper and lower bounds for λ_1 and λ_4 are summarized in table 5.1 and table 5.2 below.

	lower bound	Upper bound	Equation
λ_1	6.2149	9.2839	(5.9)
λ_4	11.5851	18.3796	(5.8)
λ_4	10.2956	20.5913	(5.11)
λ_4		20.5913	(5.16)

Table 5.1: Extremal Bounds, $\eta_1 = 7.8$ and $\eta_3 = 2\sqrt{78}$.

From the Gershgorin circle theorem[6] we know that $\sigma(Q) \in [7, 13]$.

	lower bound	Upper bound	Equation
λ_1	5.6277	8.6277	(5.9)
λ_4	11.3723	14.3723	(5.8)

Table 5.2: Extremal Bounds, $\eta_1 = 7$ and $\eta_3 = 13$.

By comparing the results in table 5.1 and table 5.2 we conclude that the tighter bounds are given by $6.2149 \leq \lambda_1 \leq 8.6277$ and $11.3723 \leq \lambda_4 \leq 14.3723$.

The result of Proposition 5.4.2 applied to the matrix in (5.21) gives $\sqrt{106} < 5 + \sqrt{31}$.

Chapter 6

Conclusion

We have shown how Hermitian matrices arise naturally in various scientific applications. We have presented the Courant-Fischer theorem which is indispensable in this regard. Various fundamental results were proved for positive definite matrices.

Lower bounds for the maximum eigenvalues of such matrices were found by applying Taylor series expansion for increasing functions. The computation of these bounds for large matrices will be expensive since it involves powers of the matrix. If fewer terms are used in the Taylor expansion then other numerical techniques can be used to improve these bounds.

Expressions for the bounds of extremal eigenvalues for positive definite Toeplitz matrices are much simpler to obtain as shown in Chapter five. A further study would be to determine upper bounds for the smallest eigenvalue of positive definite matrices.

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