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Under the Direction of Marina Arav and Frank Hall

ABSTRACT

Having origins in the increasingly popular Matrix Theory, the square root function of a matrix has received notable attention in recent years. In this thesis, we discuss some of the more common matrix functions and their general properties, but we specifically explore the square root function of a matrix and the most efficient method (Schur decomposition) of computing it. Calculating the square root of a 2×2 matrix by the Cayley-Hamilton Theorem is highlighted, along with square roots of positive semidefinite matrices and general square roots using the Jordan Canonical Form.

Keywords: Cayley-Hamilton Theorem, Interpolatory Polynomials, Jordan Canonical Form, Matrix Theory, Functions of Matrices, Positive Semidefinite Matrices, Schur's Theorem, Square Roots of Matrices

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1. Introduction

As stated in [1] and [19], the introduction and development of the notion of a matrix and the subject of linear algebra followed the development of determinants. Gottfried Leibnitz, one of the two founders of calculus, used determinants in 1693 arising from the study of coefficients of systems of linear equations. Additionally, Cramer presented his determinant-based formula, known as Cramer's Rule, for solving systems of linear equations in 1750. However, the first implicit use of matrices occurred in Lagrange's work on bilinear forms in the late 1700's in his method now known as Lagrange's multipliers. Some research indicates that the concept of a determinant first appeared between 300 BC and AD 200, almost 2000 years before its invention by Leibnitz, in the Nine Chapters of the Mathematical Art by Chiu Chang Suan Shu. There is no debate that in 1848 J.J. Sylvester coined the term, "matrix", which is the Latin word for womb, as a name for an array of numbers. Matrix algebra was nurtured by the work of Arthur Cayley in 1855. He studied compositions of linear transformations and was led to define matrix multiplication, so that the matrix of coefficients for the composite transformation AB is the product of the matrix A times the matrix B. Cayley went on to study the algebra of these compositions including matrix inverses and is famous for the Cayley-Hamilton theorem, which is presented later in this thesis.

In mathematics, a matrix is a rectangular table of numbers, or more generally, a table consisting of abstract quantities. Matrices are used to describe linear equations, keep track of coefficients of linear transformations, and to record data that depend on two parameters. Matrices can be added, multiplied, and decomposed in various ways, which makes them a key concept in linear algebra and matrix theory, two of the fundamental tools in mathematical disciplines. This makes intermediate facts about matrices necessary to understand nearly every area of mathematical science, including but not limited to differential equations, probability, statistics, and optimization. Additionally, continuous research and interest in applied mathematics created the need for the development of courses devoted entirely to another key concept, the functions of matrices.

In this thesis, we provide a detailed overview of the basic functions of matrices while focusing on the square root function of a matrix and a few of the most common computational methods. We discuss the specific case of a square root of a 2×2 matrix before outlining results on square roots of positive semidefinite matrices and general square roots.

Although the theory of matrix square roots is rather complicated, simplification occurs for certain classes of matrices. Consider, for example, symmetric positive semi(definite) matrices. Any such matrix has a unique symmetric positive semi(definite) square root, and this root finds use in the theory of the generalized eigenproblem [16] (section 15-10), and preconditioned methods [4, 10]. More generally, any matrix A having no nonpositive real eigenvalues has a unique square root, for which every eigenvalue has a positive real part, and it is this square root, denoted $A^{\frac{1}{2}}$ and sometimes called the *principal square root*, that is usually of interest (e.g. the application in boundary value problems, [17]).

There is a vast amount of references available focusing on the square root function of a matrix, many of which are listed in the References section. While some of the references were used explicitly, all provided insight and assistance in the completion of this thesis.

We begin now by defining key terms used throughout this thesis for clarity and cohesiveness.

Definitions

As in [8] and [9], we let M_n denote the set of all $n \times n$ complex matrices. We note that some authors use the notation $\mathbb{C}^{n \times n}$. Now let $A \in M_n$. Then a nonzero vector $x \in \mathbb{C}^n$ is said to be an *eigenvector* of A corresponding to the *eigenvalue* λ, if

$$Ax = \lambda x.$$

The set containing all of the eigenvalues of A is called *the spectrum of* A and is denoted, $\sigma(A)$.

Let $A, B \in M_n$. Then B is a *square root* of A, if $B^2 = A$.

A matrix $D = [d_{ij}] \in M_n$ is called a *diagonal matrix*, if $d_{ij} = 0$ whenever $i \neq j$.

Let $A, B \in M_n$. Then A is *similar* to B, denoted $A \sim B$, if there is a nonsingular matrix S such that $S^{-1}AS = B$. If $A \sim B$, then they have the same characteristic polynomial and therefore the same eigenvalues with the same multiplicities.

Let $A \in M_n$. Then A is *diagonalizable*, if A is similar to a diagonal matrix.

A matrix $U \in M_n$ is said to be *unitary*, if $U^*U = I$.

A matrix $A \in M_n$ is said to be *unitarily equivalent* or *unitarily similar* to $B \in M_n$, if there is an unitary matrix $U \in M_n$ such that $U^*AU = B$. If U may be taken to be real (and therefore real orthogonal), then A is said to be (real) *orthogonally equivalent* to B.

If a matrix $A \in M_n$ is unitarily equivalent to a diagonal matrix, A is said to be *unitarily diagonalizable*.

Let $A \in M_n$. Then A is *Hermitian*, if $A^* = A$, where $A^* = \bar{A}^T = [\bar{a}_{ji}]$. If $A \in M_n$ is Hermitian, then the following statements hold:

(a) All eigenvalues of A are real; and

(b) A is unitarily diagonalizable.

The *minimal polynomial of* A, denoted $m(t)$, is the monic annihilating polynomial of the least possible degree.

An $n \times n$ matrix A is called *upper triangular*, if $a_{ij} = 0$ for $i > j$, i.e. all of the entries below the main diagonal are zero.

An $n \times n$ matrix A is called *lower triangular*, if $a_{ij} = 0$ for $i < j$, i.e. all of the entries above the main diagonal are zero.

The functions of matrices appear widely in many areas of linear algebra and are linked to numerous applications in both science and engineering. While the most common matrix function is the matrix inverse (usually mentioned with terms: invertible or nonsingular), other general matrix functions are the matrix square root, the trigonometric, the exponential and the logarithmic functions. The following are the definitions of the matrix functions mentioned above.

Examples of General Matrix Functions

A matrix A is *invertible* or *nonsingular*, if there exists a unique *inverse* denoted by A^{-1}, where $A^{-1}A = I$ and $AA^{-1} = I$ and I is the identity matrix.

Let $p(t) = a_k t^k + \cdots + a_1 t + a_0$ be a polynomial. Then, by definition,

$$p(A) = a_k A^k + \cdots + a_1 A + a_0 I.$$

The *exponential of* $A \in M_n$, denoted e^A or $exp(A)$, is defined by

$$e^A = I + A + \frac{A^2}{2!} + \cdots + \frac{A^k}{k!} + \cdots .$$

Let $A \in M_n$. Any X such that $e^X = A$ is a *logarithm* of A.

The *sine* and *cosine* of $A \in M_n$ are defined by

$$\cos(A) = I - \frac{A^2}{2!} + \cdots + \frac{(-1)^k}{(2k)!} A^{2k} + \cdots ,$$

$$\sin(A) = A - \frac{A^3}{3!} + \cdots + \frac{(-1)^k}{(2k+1)!} A^{2k+1} + \cdots .$$

2. Functions of Matrices

We provide a detailed overview of the basic ideas of functions of matrices to aid the reader in the understanding of the "connectivity" of the fundamental principles (many of which are defined in the introduction) of matrix theory.

One can easily show that if $Ax = \lambda x$ and $p(t)$ is a polynomial, then $p(A)x = p(\lambda)x$, so that if x is an eigenvector of A corresponding to λ, then x is an eigenvector of $p(A)$ corresponding to the eigenvalue $p(\lambda)$. We will shortly obtain an even stronger result.

Perhaps the most fundamentally useful fact of elementary matrix theory is that any matrix $A \in M_n$ is unitarily equivalent to an upper triangular (also to a lower triangular) matrix T. Representing the simplest form achievable under unitary equivalence, we now recall one of the most useful theorems in all of matrix theory, Schur's Theorem.

Schur's Theorem: If $A \in M_n$, then A is unitarily triangularizable, that is, there exists a unitary matrix U and an upper-triangular matrix T such that $U^*AU = T$.

Through the use of Schur's Theorem, one can prove that if $A \in M_n$ with $\sigma(A) = \{\lambda_1, \ldots, \lambda_n\}$ and $p(t)$ is a polynomial, then

$$\sigma(p(A)) = \{p(\lambda_1), \ldots, p(\lambda_n)\}.$$

The proof goes as follows: $U^*p(A)U = p(U^*AU) = p(T)$, which is upper-triangular with $p(\lambda_1), \ldots, p(\lambda_n)$ on the diagonal. The proof follows from the similarity of $p(A)$ and $p(T)$.

We now shift our focus from polynomials to general functions.

Let $A \in M_n$ and suppose that λ_1, λ_2,..., λ_s are the distinct eigenvalues of A, so that

$$m(t) = (t - \lambda_1)^{m_1}(t - \lambda_2)^{m_2} \cdots (t - \lambda_s)^{m_s}$$

is the minimal polynomial of A with degree $m = m_1 + m_2 + \ldots + m_s$. Then m_k is the *index* of the eigenvalue λ_k, i.e. it is the size of the largest Jordan block associated with λ_k and is equal to the maximal degree of the elementary divisors associated with λ_k $(1 \leq k \leq s)$.

Now, a function $f(t)$ is *defined on the spectrum of* A, if the numbers

$$f(\lambda_k), f'(\lambda_k), \ldots, f^{(m_k-1)}(\lambda_k), \quad k = 1, 2, ..., s,$$

are defined (exist). These numbers are called the *values of* $f(t)$ *on the spectrum of* A, where if $m_k = 1$, $f^{(m_k-1)}$ is $f^{(0)}$ or simply f.

Many of the succeeding results can be found in [12], but we will provide more details here.

Proposition 2.1: Every polynomial is defined on the spectrum of any matrix in M_n. For the polynomial $m(t)$, the values of

$$m(\lambda_k), m'(\lambda_k), ..., m^{(m_{k-1})}(\lambda_k), \quad k = 1, 2, \ldots, s,$$

are all zero.

Proof: The first statement is clear. Next, each $m(\lambda_k) = 0$. So,

$$m'(t) = (t-\lambda_1)^{m_1}\frac{d}{dt}[(t-\lambda_2)^{m_2}\cdots(t-\lambda_s)^{m_s}] + [(t-\lambda_2)^{m_2}\cdots(t-\lambda_s)^{m_s}]\cdot m_1(t-\lambda_1)^{m_1-1}.$$

Therefore,

$$m'(\lambda_1) = 0\cdot\frac{d}{dt}[(t-\lambda_2)^{m_2}\cdots(t-\lambda_s)^{m_s}] + [(t-\lambda_2)^{m_2}\cdots(t-\lambda_s)^{m_s}]\cdot 0 = 0, \text{if } m_1 > 1.$$

Similarly, for the other λ_k and the higher order derivatives. ■

Proposition 2.2: For the two polynomials $p_1(t)$ and $p_2(t)$, $p_1(A) = p_2(A)$ if and only if $p_1(t)$ and $p_2(t)$ have the same values on the spectrum of A.

Proof: $\Rightarrow$ Suppose $p_1(A) = p_2(A)$. Let $p_0(t) = p_1(t)$ - $p_2(t)$. Then, $p_0(A) = 0$. So, $m(t)$ is a factor of $p_0(t)$, i.e. $p_0(t) = q(t)m(t)$ for some polynomial $q(t)$. Now, each term of $p_0^{(j)}(t)$ is a product, which involves one of the terms:

$$m(t), m'(t), ..., m^{(j)}(t).$$

Hence, by Proposition 2.1,

$$p_1^{(j)}(\lambda_k) - p_2^{(j)}(\lambda_k) = p_0^{(j)}(\lambda_k) = 0,$$

for $j = 0, 1, ..., m_k - 1,$ and $1 \leq k \leq s$. So, $p_1^{(j)}(\lambda_k) = p_2^{(j)}(\lambda_k)$ for the values of j and k.

$\Leftarrow$ We assume that $p_1(t)$ and $p_2(t)$ have the same values on the spectrum of A. Let $p_0(t) = p_1(t) - p_2(t)$, then

$$p_0^{(j)}(\lambda_k) = 0 \text{ for } j = 0, 1, 2, ..., m_k - 1.$$

So, λ_k is a zero of $p_0(t)$ with multiplicity of at least m_k, i.e. $(t - \lambda_k)^{m_k}$ is a factor of $p_0(t)$. Hence, $m(t)$ is a factor of $p_0(t)$, where $p_0(t) = q(t)m(t)$ and therefore, $p_0(A) = 0$. Thus, $p_1(A) = p_2(A)$. $\blacksquare$

Proposition 2.3 (Interpolatory Polynomial): Given distinct numbers $\lambda_1, \lambda_2, \ldots, \lambda_s$, positive integers $m_1, m_2, \ldots, m_s$ with $m = \sum_{k=1}^{s} m_k$, and a set of numbers

$$f_{k,0}, \quad f_{k,1}, \ldots, \quad f_{k,m_k-1}, \; k = 1, 2, \ldots, s,$$

there exists a polynomial $p(t)$ of degree less than m such that

$$p(\lambda_k) = f_{k,0}, \quad p^{(1)}(\lambda_k) = f_{k,1}, \; \ldots, \quad p^{(m_k-1)}(\lambda_k) = f_{k,m_k-1} \text{ for } k = 1, 2, \ldots, s. \quad (1)$$

Proof: It is easily seen that the polynomial $p_k(t) = \alpha_k(t)\psi_k(t)$ (note: if $s = 1$, then by definition $\psi_1(t) \equiv 1$), where $1 \leq k \leq s$ and

$$\alpha_k(t) = \alpha_{k,0} + \alpha_{k,1}(t - \lambda_k) + \cdots + \alpha_{k,m_k-1}(t - \lambda_k)^{m_k-1},$$

$$\psi_k(t) = \prod_{j=1, j\neq k}^{s} (t-\lambda_j)^{m_j},$$

has degree less than m and satisfies the conditions

$$p_k(\lambda_i) = p_k^{(1)}(\lambda_i) = \cdots = p_k^{(m_i-1)}(\lambda_i) = 0$$

for $i \neq k$ and arbitrary $\alpha_{k,0}, \alpha_{k,1}, \cdots, \alpha_{k,m_k-1}$. Hence, the polynomial

$$p(t) = p_1(t) + p_2(t) + \cdots + p_s(t) \tag{2}$$

satisfies conditions (1) if and only if

$$p_k(\lambda_k) = f_{k,0}, \quad p_k^{(1)}(\lambda_k) = f_{k,1}, \ \ldots, \quad p_k^{(m_k-1)}(\lambda_k) = f_{k,m_k-1} \text{ for each } 1 \leq k \leq s. \tag{3}$$

By differentiation,

$$p_k^{(j)}(\lambda_k) = \sum_{i=0}^{j} \binom{j}{i} \alpha_k^{(i)}(\lambda_k)\psi_k^{(j-i)}(\lambda_k)$$

for $1 \leq k \leq s,\ 0 \leq j \leq m_k - 1$. Using Eqs.(3) and recalling the definition of $\alpha_k(\lambda)$, we have for $k = 1, 2, \ldots, s,\ j = 0, 1, \ldots, m_k - 1$,

$$f_{k,j} = \sum_{i=0}^{j} \binom{j}{i} i!\alpha_{k,i}\psi_k^{(j-i)}(\lambda_k). \tag{4}$$

Since $\psi_k(\lambda_k) \neq 0$ for each fixed k, Eqs. (4) can now be solved successively (beginning with $j = 0$) to find the coefficients $\alpha_{k,0}, \ldots, \alpha_{k,m_k-1}$ for which (3) holds. Thus, a polynomial $p(t)$ of the form given in (2) satisfies the required conditions. $\blacksquare$

The interpolatory polynomial referred to in Proposition 2.3 is known as the *Hermite interpolating polynomial*. It is in fact unique, but the proof of the uniqueness is omitted, since it is quite cumbersome. If $f(t)$ is defined on the spectrum of A, we define $f(A)$ to be $p(A)$, where $p(t)$ is the interpolating polynomial for $f(t)$ on the spectrum of A.

Theorem 2.4: If $A \in M_n$ is a block-diagonal matrix,

$$A = \text{diag}[A_1, A_2, ..., A_t],$$

and the function $f(t)$ is defined on the spectrum of A, then

$$f(A) = \text{diag}[f(A_1), f(A_2), ..., f(A_t)]. \tag{5}$$

Proof: It is clear that for any polynomial $q(t)$,

$$q(A) = \text{diag}[q(A_1), q(A_2), ..., q(A_t)].$$

Hence, if $p(t)$ is the interpolatory polynomial for $f(t)$ on the spectrum of A, we have

$$f(A) = p(A) = \text{diag}[p(A_1), p(A_2), ..., p(A_t)].$$

Since the spectrum of A_j $(1 \le j \le t)$ is obviously a subset of the spectrum of A, the function $f(t)$ is defined on the spectrum of A_j for each $j = 1, 2, ..., t$. (Note also that the index of an eigenvalue of A_j cannot exceed the index of the same eigenvalue of A.) Furthermore, since $f(t)$ and $p(t)$ assume the same values on the spectrum of A, they must also have the same values on the spectrum of A_j $(j = 1, 2, ..., t)$. Hence,

$$f(A_j) = p(A_j)$$

and we obtain Eq. (5). ■

Theorem 2.5: If $A, B, S \in M_n$, where $B = SAS^{-1}$, and $f(t)$ is defined on the spectrum of A, then

$$f(B) = Sf(A)S^{-1}. \tag{6}$$

Proof: Since A and B are similar, they have the same minimal polynomial. Thus, if $p(t)$ is the interpolatory polynomial for $f(t)$ on the spectrum of A, then it is also the interpolatory polynomial for $f(t)$ on the spectrum of B. Thus, we have

$$f(A) = p(A),$$

$$f(B) = p(B),$$

$$p(B) = Sp(A)S^{-1},$$

so the relation (6) follows. ■

Theorem 2.6: Let $A \in M_n$ and let $J = \text{diag}[J_j]_{j=1}^t$ be the Jordan canonical form of A, where $A = SJS^{-1}$ and J_j is the j^{th} Jordan block of J. Then

$$f(A) = S\ \text{diag}[f(J_1), f(J_2), ..., f(J_t)]S^{-1}. \tag{7}$$

The last step in computing $f(A)$ by use of the Jordan form of A consists of the following formula.

Theorem 2.7: Let J_0 be a Jordan block of size l associated with λ_0:

$$J_0 = \begin{bmatrix} \lambda_0 & 1 & & \\ & \lambda_0 & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_0 \end{bmatrix}.$$

If $f(t)$ is an $(l-1)$-times differentiable function in a neighborhood of λ_0, then

$$f(J_0) = \begin{bmatrix} f(\lambda_0) & \frac{1}{1!}f'(\lambda_0) & \dots & \frac{1}{(l-1)!}f^{(l-1)}(\lambda_0) \\ 0 & f(\lambda_0) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{1}{1!}f'(\lambda_0) \\ 0 & \dots & 0 & f(\lambda_0) \end{bmatrix}. \tag{8}$$

Proof: The minimal polynomial of J_0 is $(t - \lambda_0)^l$ and the values of $f(t)$ on the spectrum of J_0 are therefore $f(\lambda_0)$, $f'(\lambda_0)$,$\dots$,$f^{(l-1)}(\lambda_0)$. The interpolatory polynomial $p(t)$, defined by the values of $f(t)$ on the spectrum $\{\lambda_0\}$ of J_0, is found by putting $s = 1, m_k = 1, \lambda_1 = \lambda_0$, and $\psi_1(t) \equiv 1$. One obtains

$$p(t) = \sum_{i=0}^{l-1} \frac{1}{i!} f^{(i)}(\lambda_0)(t - \lambda_0)^i.$$

The fact that the polynomial $p(t)$ solves the interpolation problem $p^{(j)}(\lambda_0) = f^{(j)}(\lambda_0), 1 \leq j \leq l-1$, can also be easily checked by a straightforward calculation.

We then have $f(J_0) = p(J_0)$ and hence

$$f(J_0) = \sum_{i=0}^{l-1} \frac{1}{i!} f^{(i)}(\lambda_0)(J_0 - \lambda_0 I)^i.$$

Computing the powers of $J_0 - \lambda_0 I$, we obtain

$$(J_0 - \lambda_0 I)^i = \begin{bmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{bmatrix}^i = \begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ & & & & & \ddots & \vdots \\ & & & & \ddots & & 0 \\ & & & & \ddots & & 1 \\ & & & & & & 0 \\ & & & & & & \vdots \\ & & & & & & 0 \end{bmatrix}$$

with 1's in the i-th super-diagonal positions, and zeros elsewhere, and Eq.(8) follows.

■

Thus, given a Jordan decomposition of the matrix A, the matrix $f(A)$ is easily found by combining Theorems 2.6 and 2.7.

From Theorems 2.6 and 2.7, we have the following results.

Theorem 2.8: Using the notation of Theorem 2.6,

$$f(A) = S \ \mathrm{diag}[f(J_1), f(J_2), ..., f(J_t)]S^{-1},$$

where $f(J_i)$ $(i = 1, 2, ..., t)$ are upper triangular matrices of the form given in Eq.(8).

Theorem 2.9: If $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of the matrix $A \in M_n$ and $f(t)$ is defined on the spectrum of A, then the eigenvalues of $f(A)$ are $f(\lambda_1), f(\lambda_2), ..., f(\lambda_n)$.

This follows from the fact that the eigenvalues of an upper triangular matrix are its diagonal entries.

3. The Square Root of a 2×2 Matrix

If $A, B \in M_n$ and A is similar to B, then A has a square root if and only if B has a square root. The standard method for computing a square root of an $n \times n$ diagonalizable matrix A is easily stated. Suppose

$$S^{-1}AS = D$$

for some nonsingular matrix S and diagonal matrix D. Then

$$A = SDS^{-1},$$

and by substitution we have

$$A = (S\hat{D}S^{-1})(S\hat{D}S^{-1}) = SDS^{-1},$$

where $\hat{D}$ is a square root of D. In general, the matrix D will have 2^n distinct square roots (when A has n nonzero eigenvalues, which are obtained by taking the square roots of the diagonal elements of D with all possible sign choices). If $D^{1/2}$ is any square root of D, it follows that $B = SD^{1/2}S^{-1}$ is a square root of A, that is $B^2 = A$. However, even in some 2×2 cases, the computations can become quite messy.

Not every 2×2 matrix has a square root. For example, by direct calculation, we can show that

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

has no square root. On the other hand, if $b \in \mathbb{C}$,

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

gives an infinite number of square roots of

$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

and if $b \neq 1$,

$$\frac{1}{b-1}\begin{bmatrix} b & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & -1 \\ -1 & b \end{bmatrix} = \frac{1}{b-1}\begin{bmatrix} -b-1 & 2b \\ -2 & b+1 \end{bmatrix}$$

yields an infinite number of square roots of

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

We next recall another useful theorem in matrix analysis, the Cayley-Hamilton Theorem.

Cayley-Hamilton Theorem: If $A \in M_n$ and $p_A(t) = \det(tI - A)$ is the characteristic polynomial of A, then $p_A(A) = 0$.

In [15] and [18], the authors show how the Cayley-Hamilton Theorem may be used to determine explicit formulae for all the square roots of 2×2 matrices. These formulae indicate exactly when a 2×2 matrix has square roots, and the number of such roots. Suppose A is 2×2 and

$$X^2 = A. \tag{9}$$

However, for each 2×2 matrtix X, the Cayley-Hamilton Theorem states that

$$X^2 - (\mathrm{trX})\mathrm{X} + (\det \mathrm{X})\mathrm{I} = 0. \tag{10}$$

Thus, if a 2×2 matrix A has a square root X, then we may use (10) to eliminate X^2 from (9) to obtain

$$\mathrm{tr}(\mathrm{X})\mathrm{X} = \mathrm{A} + (\det \mathrm{X})\mathrm{I}.$$

Now, since $(\det X)^2 = \det X^2 = \det A$, then

$$\det X = \epsilon_1 \sqrt{\det A}, \quad \epsilon_1 = \pm 1,$$

that is $\det \sqrt{A} = \epsilon_1 \sqrt{\det A}$, so that the above result simplifies to the identity:

$$(\mathrm{trX})\mathrm{X} = \mathrm{A} + \epsilon_1 \sqrt{\det \mathrm{A}}\mathrm{I}, \;\; \epsilon_1 = \pm 1. \tag{11}$$

Case 1: A is a scalar matrix. If A is a scalar matrix, $A = aI$, then (11) gives

$$(\mathrm{trX})\mathrm{X} = (1 + \epsilon_1)\mathrm{aI}, \ \epsilon_1 = \pm 1.$$

Hence, either $(\mathrm{trX})\mathrm{X} = 0$, or $(\mathrm{trX})\mathrm{X} = 2\mathrm{aI}$. The first of these possibilities determines the general solution of (9) as

$$X = \begin{pmatrix} \alpha & \beta \\ \gamma & -\alpha \end{pmatrix}, \ \alpha^2 + \beta\gamma = a, \tag{12}$$

and it covers the second possibility, if $a = 0$. On the other hand, if $a \neq 0$, then the second possibility, $(\mathrm{trX})\mathrm{X} = 2\mathrm{aI}$, implies X is scalar and has only one pair of solutions

$$X = \pm\sqrt{a}I. \tag{13}$$

For this case, we conclude that if A is a zero matrix, then it has a double-infinity of square roots as given by (12) with $a = 0$, whereas if A is a nonzero, scalar matrix, then it has a double-infinity of square roots plus two scalar square roots as given by (12) and (13).

Case 2: A is not a scalar matrix. If A is not a scalar matrix, then $\mathrm{trX} \neq 0$ in (11). Consequently, every square root X has the form:

$$X = \tau^{-1}(A + \epsilon_1\sqrt{\det A}I), \ \tau \neq 0.$$

Substituting this expression for X into (9) and using the Cayley-Hamilton theorem for A, we find

$$A^2 + (2\ \epsilon_1\sqrt{\det A} - \tau^2)A + (\det A)I = 0$$

$$((\mathrm{trA})\mathrm{A} - (\det \mathrm{A})\mathrm{I}) + (2\ \epsilon_1\sqrt{\det \mathrm{A}} - \tau^2)\mathrm{A} + (\det \mathrm{A})\mathrm{I} = 0$$

$$(trA + 2\ \epsilon_1\sqrt{\det A} - \tau^2)A = 0.$$

Since A is not a scalar matrix, then A is not a zero matrix, so

$$\tau^2 = trA + 2\ \epsilon_1\sqrt{\det A}, \ (\tau \neq 0, \ \epsilon_1 = \pm 1). \tag{14}$$

If $(\mathrm{trA})^2 \neq 4\det\mathrm{A}$, then both values of ϵ_1 may be used in (14) without reducing τ to zero. Consequently, it follows from (11) that we may write X, the square root of A, as

$$X = \epsilon_2 \frac{A + \epsilon_1\sqrt{\det A}I}{\sqrt{trA + 2\ \epsilon_1\sqrt{\det A}}}. \tag{15}$$

Here each $\epsilon_i = \pm 1$, and if $\det A \neq 0$, the result determines exactly four square roots for A. However, if $\det A = 0$, then the result (15) determines two square roots for A as given by

$$X = \pm\frac{1}{\sqrt{\mathrm{trA}}}\ A. \tag{16}$$

Alternatively, if $(trA)^2 = 4\det A \neq 0$, then one value of ϵ_1 in (14) reduces τ to zero, whereas the other value yields the results $2\epsilon_1\sqrt{\det A} = \mathrm{trA}$ and $\tau^2 = 2\ \mathrm{trA}$. In this case, A has exactly two square roots given by

$$X = \pm\frac{1}{\sqrt{2\ trA}}(A + \frac{1}{2}(trA)I). \tag{17}$$

Finally, if $(\mathrm{trA})^2 = 4\det\mathrm{A} = 0$, then both values of ϵ_1 reduce τ to zero in (14). Hence it follows by contradiction that A has no square roots.

For this case, we conclude that a nonscalar matrix, A, has square roots, if and only if, at least one of the numbers, trA and $\det A$, is nonzero. Then the matrix has four square roots given by (15), if

$$(\mathrm{trA})^2 \neq 4\det\mathrm{A},\ \det\mathrm{A} \neq 0$$

and two square roots given by (16) or (17), if

$$(\mathrm{trA})^2 \neq 4\det\mathrm{A},\ \det\mathrm{A} = 0 \text{ or } (\mathrm{trA})^2 = 4\det\mathrm{A},\ \det\mathrm{A} \neq 0.$$

It is worth noting from (15) that

$$\mathrm{tr\ X} = \mathrm{tr}\sqrt{\mathrm{A}} = \epsilon_2\sqrt{\mathrm{trA} + 2\ \epsilon_1\sqrt{\det\mathrm{A}}}.$$

Hence using the identity, $\det \sqrt{A} = \epsilon_1 \sqrt{\det A}$ as applied in (11), result (15) may be rewritten as

$$\sqrt{A} = \frac{1}{tr\sqrt{A}}(A + \det \sqrt{A} I),$$

which is equivalent to the Cayley-Hamilton Theorem for the matrix $\sqrt{A}$. This same deduction can be made, of course, for all other cases under which $\sqrt{A}$ exists.

In [2], the author is concerned with the determination of algebraic formulas yielding all of the solutions of the matrix equation $B^n = A$, where n is a positive integer greater than 2 and A is a 2×2 matrix with real or complex elements. If A is a 2×2 scalar matrix, the equation $B^n = A$ has infinitely many solutions, and one can obtain the explicit formulas giving all of the solutions. If A is a non-scalar matrix, the equation $B^n = A$ has only a finite number of solutions. While the author's concern is beyond the scope of this thesis, it outlines a process for obtaining other roots with expressed preciseness.

4. Positive Semidefinite Matrices

By definition, an $n \times n$ Hermitian matrix A is called *positive semidefinite*, if

$$x^*Ax \geq 0 \text{ for all nonzero } x \in \mathbb{C}^n.$$

Theorem 4.1: A Hermitian matrix $A \in M_n$ is positive semidefinite if and only if all of its eigenvalues are nonnegative.

Proof: Since A is Hermitian, there exists a unitary matrix U and a diagonal matrix D such that $U^*AU = D$. Then

$$x^*Ax = x^*UDU^*x = y^*Dy = \sum_{i=1}^{n} d_i \bar{y}_i y_i = \sum_{i=1}^{n} d_i |y_i|^2,$$

where $U^*x = y$.

$\Rightarrow$ Let the Hermitian matrix $A \in M_n$ be positive semidefinite. Then, from the above,

$$\sum_{i=1}^{n} d_i |y_i|^2 \geq 0, \text{for all } y \in \mathbb{C}^n.$$

Letting $y = e_i$, then $y^*Dy = d_i$. Hence, all of the eigenvalues of A are nonnegative.

$\Leftarrow$ Let $A \in M_n$ be a Hermitian matrix and suppose that all $\lambda_i(A) \geq 0$. Then

$$\sum_{i=1}^{n} d_i |y_i|^2 \geq 0$$

and hence, $x^*Ax \geq 0$ for all $x \in \mathbb{C}^n$. ■

Corollary 4.2: If $A \in M_n$ is positive semidefinite, then so are all the powers A^k, $k = 1, 2, 3, ...$

Proof: If the eigenvalues of A are λ_1, λ_2,..., λ_n, then the eigenvalues of A^k are ${\lambda_1}^k$, ${\lambda_2}^k$,..., ${\lambda_n}^k$. ■

A positive semidefinite matrix can have more than one square root. However, it can only have one positive semidefinite matrix square root. The proof of the following result is adapted from [8].

Theorem 4.3: Let $A \in M_n$ be positive semidefinite and let $k \geq 1$ be a given integer. Then there exists a unique positive semidefinite Hermitian matrix B such that $B^k = A$. We also have

(a) $BA = AB$ and there is a polynomial $p(t)$ such that $B = p(A)$;

(b) rank $B =$ rank A, so B is a positive definite if A is; and

(c) B is real if A is real.

Proof: We know that the Hermitian matrix A can be unitarily diagonalized as $A = UDU^*$ with $D = \text{diag}(\lambda_1, \lambda_2, ..., \lambda_n)$ and all $\lambda_i \geq 0$. We define $B = UD^{\frac{1}{k}}U^*$, where $D^{1/k} \equiv \text{diag}(\lambda_1^{1/k}, \lambda_2^{1/k}, ..., \lambda_n^{1/k})$, and the unique nonnegative kth root is taken in each case. Clearly, $B^k = A$ and B is Hermitian and positive semidefinite. Also, $AB = UDU^*UD^{\frac{1}{k}}U^* = UDD^{\frac{1}{k}}U^* = UD^{\frac{1}{k}}DU^* = UD^{\frac{1}{k}}U^*UDU^* = BA$, and B is positive semidefinite because all λ_i (and hence their kth roots) are nonnegative. The rank of B is just the number of nonzero λ_i terms, which is also the rank of A. If A is real and positive semidefinite, then we know that U may be chosen to be a real orthogonal matrix, so it is clear that B can be chosen to be real in this case. It remains only to consider the question of uniqueness.

Notice first that there is a polynomial $p(t)$ such that $p(A) = B$; we need only choose $p(t)$ the Lagrange interpolating poynomial for the set $\{(\lambda_1, \lambda_1^{\frac{1}{k}}), \ldots, (\lambda_n, \lambda_n^{\frac{1}{k}})\}$ to get $p(D) = D^{\frac{1}{k}}$ and $p(A) = p(UDU^*) = Up(D)U^* = UD^{\frac{1}{k}}U^* = B$. But then if C is any positive semidefinite Hermitian matrix such that $C^k = A$, we have $B = p(A) = p(C^k)$ so that $CB = Cp(C^k) = p(C^k)C = BC$. Since B and C are commuting Hermitian matrices, they may be simultaneously unitarily diagonalized; that is, there is some unitary matrix V and diagonal matrices D_1 and D_2 with nonnegative diagonal entries such that $B = VD_1V^*$ and $C = VD_2V^*$. Then from the fact that $B^k = A = C^k$ we deduce that $D_1^k = D_2^k$. But since the nonnegative kth root of a nonnegative number is unique, we conclude that $(D_1^k)^{\frac{1}{k}} = D_1 = D_2 = (D_2^k)^{\frac{1}{k}}$ and $B = C$. ■

The most useful case of the preceding theorem is for $k = 2$. The unique positive (semi)definite square root of the positive (semi)definite matrix A is usually denoted by $A^{\frac{1}{2}}$. Similarly, $A^{\frac{1}{k}}$ denotes the unique positive (semi)definite kth root of A for each $k = 1, 2, \ldots$.

An $n \times n$ Hermitian matrix A is called *positive definite*, if

$$x^*Ax > 0 \text{ for all nonzero } x \in \mathbb{C}^n.$$

If A is a real symmetric positive definite matrix, then A can be factored into a product LDL^T, where L is a lower triangular matrix with 1's along the diagonal and D is a diagonal matrix, whose diagonal entries are all positive. Then $A = (LD^{\frac{1}{2}})(D^{\frac{1}{2}}L^T)$, which is the Cholesky Decomposition of A. It is worth noting that many applications can be recast to use a Cholesky Decomposition instead of the square root. The Cholesky Decomposition becomes referred to as a square root decomposition and has many applications such as in multiwavelet representations, predictive control, and square-root filters.

5. General Square Roots

Our main tool in this chapter is the Jordan Canonical Form.

Theorem 5.1 (Jordan Form Theorem): Let $A \in M_n$. Then there is a nonsingular matrix S such that $S^{-1}AS = J$ is a direct sum of Jordan blocks. Furthermore, J is unique up to a permutation of the Jordan blocks.

Let $A = SJS^{-1}$ be the Jordan canonical form of the given matrix A, so that if $X^2 = A = SJS^{-1}$, then $S^{-1}X^2S = (S^{-1}XS)^2 = J$. It suffices, therefore, to solve the equation $X^2 = J$. But if X is such that the Jordan canonical form of X^2 is equal to J, then there is some nonsingular T such that $J = TX^2T^{-1} = (TXT^{-1})^2$. Thus, it suffices to find an X such that the Jordan canonical form of X^2 is equal to J. If the Jordan canonical form of X itself is J_X, then the Jordan canonical form of X^2 is the same as that of $(J_X)^2$, so it suffices to find a Jordan matrix J_X such that the Jordan canonical form of $(J_X)^2$ is equal to J. Finally, if $J_X = J_{m_1}(\mu_1) \oplus \cdots \oplus J_{m_r}(\mu_r)$, then the Jordan canonical form of $(J_X)^2$ is the same as the direct sum of the Jordan canonical forms of $J_{m_i}(\mu_i)^2, i = 1, \ldots, r$. Thus, to solve $X^2 = A$, it suffices to consider only whether there are choices of scalars μ and positive intergers m such that the given Jordan canonical form J is the direct sum of the Jordan canonical forms of matrices of the form $J_m(\lambda)^2$. If $\mu \neq 0$, we know that the Jordan canonical form of $J_m(\mu)^2$ is $J_m(\mu^2)$, so every nonsingular Jordan block $J_k(\lambda)$ has a square root; in fact, it has square roots that lie in two distinct similarity classes with Jordan canonical forms $J_k(\pm\sqrt{\lambda})$. If necessary, these square roots of Jordan blocks can be computed explicitly.

Thus, every nonsingular matrix $A \in M_n$ has a square root, and it has square roots in at least 2^μ different similarity classes, if A has μ distinct eigenvalues. It has square roots in at most 2^ν different similarity classes, if the Jordan canonical form of A is the direct sum of ν Jordan blocks; there are exactly 2^ν similarity classes, if all the Jordan blocks with the same eigenvalue have different sizes, but there are fewer than 2^ν, if two or more blocks of the same size have the same eigenvalue, since permuting blocks does not change the similarity class of a Jordan canonical form. Some of these nonsimilar square roots may not be "functions" of A, however. If each of the ν blocks has a different eigenvalue (i.e., A is nonderogatory), a Lagrange-Hermite interpolation polynomial can always be used to express any square root of A as a polynomial in A. If the same eigenvalue λ occurs in two or more blocks, however, polynomial interpolation is possible only if the same choice is made for $\lambda^{\frac{1}{2}}$ for all of them; if different choices are made in this case, one obtains a square root of A that is not a "function" of A in the sense that it cannot be obtained as a polynomial in A, and therefore cannot be a primary matrix function $f(A)$ with a single-valued function $f(\cdot)$.

What happens if A is singular? Since each nonsingular Jordan block of A has a square root, it suffices to consider the direct sum of all the singular Jordan blocks of A. If A has a square root, then this direct sum is the Jordan canonical form of the square of a direct sum of singular Jordan blocks. Which direct sums of singular Jordan blocks can arise in this way?

Let $k > 1$. We know that the Jordan canonical form of $J_k(0)^2$ consists of exactly two Jordan blocks $J_{k/2}(0) \oplus J_{k/2}(0)$ if $k > 1$ is even, and it consists of exactly two Jordan blocks $J_{(k+1)/2}(0) \oplus J_{(k-1)/2}(0)$ if $k > 1$ is odd.

If $k = 1$, $J_1(0)^2 = [0]$ is a 1-by-1 block, and this is the only Jordan block that is similar to the square of a singular Jordan block.

Putting together this information, we can determine whether or not a given singular Jordan matrix J has a square root as follows: Arrange the diagonal blocks of J by decreasing size, so $J = J_{k_1}(0) \oplus J_{k_2}(0) \oplus \cdots \oplus J_{k_p}(0)$ with $k_1 \geq k_2 \geq k_3 \geq \cdots \geq k_p \geq 1$. Consider the differences in sizes of successive pairs of blocks: $\Delta_1 = k_1 - k_2, \Delta_3 = k_3 - k_4, \Delta_5 = k_5 - k_6$, etc., and suppose J is the Jordan canonical form of the square of a singular Jordan matrix $\tilde{J}$. We have seen that $\Delta_1 = 0$ or 1 because either $k_1 = 1$ [in which case $J_1(0) \oplus J_1(0)$ corresponds to $(J_1(0) \oplus J_1(0))^2$ or to $J_2(0)^2$] or $k_1 > 1$ and $J_{k_1}(0) \oplus J_{k_2}(0)$ corresponds to the square of the largest Jordan block in $\tilde{J}$, which has size $k_1 + k_2$. The same reasoning shows that $\Delta_3, \Delta_5, \ldots$ must all have the value 0 or 1 and an acceptable square root corresponding to the pair $J_{k_i}(0) \oplus J_{k_{i+1}}(0)$ is $J_{k_i + k_{i+1}}(0), i = 1, 3, 5, \ldots$. If p (the total number of singular Jordan blocks in J) is odd, then the last block $J_{k_p}(0)$ is left unpaired in this process and must therefore have size 1 since it must be the square of a singular Jordan block. Conversely, if the successive differences (and k_p, if p is odd) satisfy these conditions, then the pairing process described constructs a square root for J.

Suppose $A \in M_n$ is singular and suppose there is a polynomial $r(t)$ such that $B = r(A)$ is a square root of A. Then $r(0) = 0,\ r(t) = tg(t)$ for some polynomial $g(t)$, and $A = B^2 = A^2 g(A)^2$, which is clearly impossible if rank $A^2 <$ rank A. Thus, rank $A =$ rank A^2 in this case, which means that every singular Jordan block of A is 1-by-1. Conversely, if A is singular and has minimal polynomial $q_A(t) = t(t - \lambda_1)^{r_1} \cdots (t - \lambda_\mu)^{r_\mu}$ with distinct nonzero $\lambda_1, \ldots, \lambda_\mu$ and all $r_i \geq 1$, let $g(t)$ be a polynomial that interpolates the function $f(t) = 1/\sqrt{t}$ and its derivatives at the (necessarily nonzero) roots of the polynomial $q_A(t)/t = 0$, and let $r(t) \equiv tg(t)$. For each nonsingular Jordan block $J_{n_i}(\lambda_i)$ of A, $g(J_{n_i}(\lambda_i)) = [J_{n_i}(\lambda_i)]^{-\frac{1}{2}}$ and hence, we have $r(J_{n_i}(\lambda_i)) = J_{n_i}(\lambda_i)[J_{n_i}(\lambda_i)]^{-\frac{1}{2}} = J_{n_i}(\lambda_i)^{\frac{1}{2}}$. Since all the singular Jordan blocks of A are 1-by-1 and $r(0) = 0$, we conclude that $r(A)$ is a square root of A. Thus, a given singular $A \in M_n$ has a square root that is a polynomial in A if and only if rank $A =$ rank A^2. Since this latter condition is trivially satisfied if A is nonsingular (in which case we already know that A has a square root that is a polynomial in A), we conclude that a given $A \in M_n$ has a square root that is a polynomial in A if and only if rank $A =$ rank A^2.

If we agree that a "square root" of a matrix $A \in M_n$ is any matrix $B \in M_n$ such that $B^2 = A$, we can summarize what we have learned about the solutions of the equation $X^2 - A = 0$ in Theorem 5.2.

Theorem 5.2: Let $A \in M_n$ be given.

(a) If A is nonsingular and has μ distinct eigenvalues and ν Jordan blocks in its Jordan canonical form, it has at least 2^μ and at most 2^ν nonsimilar square roots. Furthermore, at least one of its square roots can be expressed as a polynomial in A.

(b) If A is singular and has Jordan canonical form $A = SJS^{-1}$, let $J_{k_1}(0) \oplus J_{k_2}(0) \oplus \cdots \oplus J_{k_p}(0)$ be the singular part of J with the blocks arranged in decreasing order of size: $k_1 \geq k_2 \geq \cdots \geq k_p \geq 1$. Define $\Delta_1 = k_1 - k_2, \Delta_3 = k_3 - k_4, \ldots$. Then A has a square root if and only if $\Delta_i = 0$ or 1 for $i = 1, 3, 5, \ldots$ and, if p is odd, k_p =1. Furthermore, A has a square root that is a polynomial in A if and only if $k_1 = 1$, a condition that is equivalent to requiring that rank $A =$ rank A^2.

(c) If A has a square root, its set of square roots lies in finitely many different similarity classes.

Since the sizes and numbers of the Jordan blocks $J_k(\lambda)$ of a matrix A can be inferred from the sequence of ranks of the powers $(A - \lambda I)^k, k = 1, 2, \ldots,$ the necessary and sufficient condition on the sizes of the singular Jordan blocks of A in part (b) of the preceding theorem can be restated in terms of ranks of powers. Let $A \in M_n$ be a given singular matrix, and let $r_0 = n,\ r_k = rank\ A^k$ for $k = 1, 2, \ldots$. The sequence $r_0, r_1, r_2, \ldots$ is decreasing and eventually becomes constant. If $r_{k_1-1} > r_{k_1} = r_{k_1+1} = \ldots$, then the largest singular Jordan block in A has size k_1, which is the *index of the matrix with respect to the eigenvalue* $\lambda = 0$. The difference

$r_{k_1-1} - r_{k_1}$ is the number of singular Jordan blocks of size k_1. If this number is even, the blocks of size k_1 can all be paired together in forming a square root. If this number is odd, then one block is left over after the blocks are paired and A can have a square root only if either $k_1 = 1$ (so that no further pairing is required), or there is at least one singular Jordan block of size $k_1 - 1$ available to be paired with it; this is the case only if $r_{k_1-2} - r_{k_1-1} > r_{k_1-1} - r_{k_1}$, since $r_{k_1-2} - r_{k_1-1}$ equals the total number of singular Jordan blocks of sizes k_1 and $k_1 - 1$. This reasoning is easily continued backward through the sequence of ranks r_k. If all the differences $r_i - r_{i+1}$ are even, $i = k_1 - 1, k_1 - 3, \ldots$, then A has a square root. If any difference $r_i - r_{i+1}$ is odd, then $r_{i-1} - r_i$ must have a larger value, if A is to have a square root. Since $r_0 - r_1$ is the total number of singular Jordan blocks of all sizes, if $r_0 - r_1$ is odd, we must also require that there be at least one block of size 1, that is, $1 \leq$ (# of singular blocks of all sizes ≥ 1) – (# of singular blocks of all sizes ≥ 2) $= (r_0 - r_1) - (r_1 - r_2) = r_0 - 2r_1 + r_2$. Notice that $r_k \equiv$ n, if A is nonsingular, so all the successive differences $r_i - r_{i+1}$ are zero and A trivially satisfies the criteria for a square root in this case.

This theorem largely results from [3] but is presented more clearly in [9].

Corollary 5.3: Let $A \in M_n$ and let $r_0 = n, r_k =$ rank A^k for $k = 1, 2, \ldots$. Then A has a square root if and only if the sequence

$$\{r_k - r_{k+1}\},\ k = 0, 1, 2, \ldots$$

does not contain two successive occurrences of the same odd integer and, if $r_0 - r_1$ is odd, $r_0 - 2r_1 + r_2 \geq 1$.

As mentioned in chapter 3, we can use direct calculation to show that there is no matrix

$$B = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

such that

$$B^2 = A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

We can also use the criteria in Theorem 5.2 and Corollary 5.3 given by [9] to show that no such matrix B exist.

Although we now know exactly when a given complex matrix has a complex square root, one sometimes needs to answer a slightly different question: When does a given real matrix $A \in M_n(\mathbb{R})$ have a real square root? The equivalent criteria in Theorems 5.2 and Corollary 5.3 are still necessary, of course, but they do not guarantee that any of the possible square roots are real. The crucial observation needed here is that if one looks at the Jordan canonical form of a real matrix, then the Jordan blocks with nonreal eigenvalues occur only in conjugate pairs, i.e., there is an even number of Jordan blocks of each size for each nonreal eigenvalue. Moreover, a given complex matrix is similar to a real matrix if and only if the nonreal blocks in its Jordan canonical form occur in conjugate pairs.

If there is some $B \in M_n$ such that $B^2 = A$, then any Jordan block of A with a negative eigenvalue corresponds to a Jordan block of B of the same size with a purely imaginary eigenvalue. If B is real, such blocks must occur in conjugate pairs, which means that the Jordan blocks of A with negative eigenvalues must also occur in pairs, just like the nonreal blocks of A.

Conversely, let J be the Jordan canonical form of the real matrix $A \in M_n(\mathbb{R})$, suppose all of the Jordan blocks in J with negative eigenvalues occur in pairs, and suppose A satisfies the rank conditions in Corollary 5.3. Form a square root for J using the process leading to Theorem 5.2 for the singular blocks, and using the primary-function method (found in [9]) for each individual nonsingular Jordan block, but be careful to choose conjugate values for the square root for the two members of each pair of blocks with nonreal or negative eigenvalues; blocks or groups of blocks with nonnegative eigenvalues necessarily have real square roots. Denote the resulting, possibly complex, block diagonal upper triangular matrix by C, so $C^2 = J$. Each diagonal block of C is similar to a Jordan block of the same size with the same eigenvalue, so C is similar to a real matrix R because of the conjugate pairing of its nonreal Jordan blocks. Thus, the real matrix R^2 is similar to $C^2 = J$, and J is similar to the real matrix A, so R^2 is similar to A. Recall that two real matrices are similar if and only if they are similar via a real similarity, since they must have the same real Jordan canonical form, which can always be attained via a real similarity. Thus, there is a real nonsingular $S \in M_n(\mathbb{R})$ such that $A = SR^2S^{-1} = SRS^{-1}SRS^{-1} = (SRS^{-1})^2$ and the real matrix SRS^{-1} is therefore a real square root of A.

In the above argument, notice that if A has any pairs of negative eigenvalues, the necessity of choosing conjugate purely imaginary values for the square roots of the two members of each pair precludes any possibility that a real square root of A could be a polynomial in A or a primary matrix function of A. The following theorem summarizes these observations.

Theorem 5.4: Let $A \in M_n(\mathbb{R})$ be a given real matrix. There exists a real $B \in M_n(\mathbb{R})$ with $B^2 = A$ if and only if A satisfies the rank condition given in Corollary 5.3 and has an even number of Jordan blocks of each size for every negative eigenvalue. If A has any negative eigenvalues, no real square root of A can be a polynomial in A or a primary matrix function of A.

The same reasoning used before to analyze the equation $X^2 = A$ can be used to analyze $X^m = A$ for $m = 3, 4, \ldots$. Every nonsingular $A \in M_n$ has an mth root, in fact, a great many of them, and the existence of an mth root of a singular matrix is determined entirely by the sequence of sizes of its singular Jordan blocks.

From [11], it is important to note that if $\sigma(A) \cap (-\infty, 0] = \emptyset$, then A has a unique square root $B \in M_n$ with $\sigma(B)$ in the open right (complex) half plane.

6. Computational Method

To evaluate matrix square root functions, it is suggested that the most stable way is to use the Schur decomposition. Recalling Schur's Theorem, we know that for each complex matrix A there exist a unitary matrix q and upper triangular matrix t, such that $A = qtq^{-1}$. A square root b of the upper triangular factor t could be computed by directly solving the equation $b^2 = t$. The choices of signs on the diagonal of b, $b_{mm} = \sqrt{t_{mm}}$ determine which square root is obtained. $\{t_{mm}\}$ are eigenvalues of A, $\{b_{mm}\}$ are eigenvalues of b, and the principal $\sqrt{A}$ has nonnegative eigenvalues or eigenvalues with a nonnegative real part. Using Schur decomposition, we have

$$A = qtq^{-1},$$

$$b^2 = t,$$

$$c = qbq^{-1},$$

$$c^2 = qbq^{-1}qbq^{-1} = qb^2q^{-1} = qtq^{-1} = A.$$

The most time consuming if done by hand is Schur decomposition. Fortunately, MatLab does it for us. Computing b that satisfies $b^2 = t$ is the next time consuming (if done by hand) portion of this process. Consider the following 4×4 matrix.

$$\begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ 0 & b_{22} & b_{23} & b_{24} \\ 0 & 0 & b_{33} & b_{34} \\ 0 & 0 & 0 & b_{44} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ 0 & b_{22} & b_{23} & b_{24} \\ 0 & 0 & b_{33} & b_{34} \\ 0 & 0 & 0 & b_{44} \end{bmatrix} = \begin{bmatrix} t_{11} & t_{12} & t_{13} & t_{14} \\ 0 & t_{22} & t_{23} & t_{24} \\ 0 & 0 & t_{33} & t_{34} \\ 0 & 0 & 0 & t_{44} \end{bmatrix}.$$

Since the eigenvalues of the upper triangular matrix t are the main diagonal entries, we can use them to calculate the eigenvalues of the matrix b. First we compute entries of the main diagonal: $b_{mm} = \sqrt{t_{mm}}$, then we compute entries on the first diagonal parellel to the main one.

$$t_{12} = b_{11}b_{12} + b_{12}b_{22} = b_{12}(b_{11} + b_{22})$$

$$b_{12} = \frac{t_{12}}{b_{11} + b_{22}}$$

$$t_{23} = b_{22}b_{23} + b_{23}b_{33} = b_{23}(b_{22} + b_{33})$$

$$b_{23} = \frac{t_{23}}{b_{22} + b_{23}}$$

$$t_{34} = b_{33}b_{34} + b_{34}b_{44} = b_{34}(b_{33} + b_{44})$$

$$b_{34} = \frac{t_{34}}{b_{33} + b_{44}}$$

After that, we compute elements of the second diagonal parellel to the main one.

$$t_{13} = b_{11}b_{13} + b_{12}b_{23} + b_{13}b_{33}$$

$$t_{13} - b_{12}b_{23} = b_{13}(b_{11} + b_{33})$$

$$b_{13} = \frac{t_{13} - b_{12}b_{23}}{b_{11} + b_{33}}$$

$$t_{24} = b_{22}b_{24} + b_{23}b_{34} + b_{24}b_{44}$$

$$t_{24} - b_{23}b_{34} = b_{24}(b_{22} + b_{44})$$

$$b_{24} = \frac{t_{24} - b_{23}b_{34}}{b_{22} + b_{44}}$$

Finally, we compute elements of the third diagonal parallel to the main one. In case of the 4-th order, it consists of only one element.

$$t_{14} = b_{11}b_{14} + b_{12}b_{24} + b_{13}(b_{34} + b_{14}b_{44})$$

$$t_{14} - b_{12}b_{24} - b_{13}b_{34} = b_{14}(b_{11} + b_{44})$$
$$b_{14} = \frac{t_{14} - b_{12}b_{24} - b_{13}b_{34}}{b_{11} + b_{44}}.$$

Therefore, we have

$$b_{12} = \frac{t_{12}}{b_{11} + b_{22}},$$

$$b_{23} = \frac{t_{23}}{b_{22} + b_{23}},$$

$$b_{34} = \frac{t_{34}}{b_{33} + b_{44}},$$

$$b_{13} = \frac{t_{13} - b_{12}b_{23}}{b_{11} + b_{33}},$$

$$b_{24} = \frac{t_{24} - b_{23}b_{34}}{b_{22} + b_{44}},$$

$$b_{14} = \frac{t_{14} - b_{12}b_{24} - b_{13}b_{34}}{b_{11} + b_{44}}.$$

Now we can derive the following algorithm for a matrix of n-th order.

For $m = 1, 2, \ldots, n:$

$$b_{mm} = \sqrt{t_{mm}}$$

For $m = 1, 2, \ldots, n - 1:$

$$b_{m,m+1} = \frac{t_{m,m+1}}{b_{m,m} + b_{m+1,m+1}}$$

For $r = 2, 3, \ldots, n-1$ and $m = 1, 2, \ldots, n-r$:

$$b(m, m+r) = \frac{t(m, m+r) - \displaystyle\sum_{k=m+1}^{m+r+1} b(m,k) \cdot b(k, m+r)}{b_{m,m} + b_{m+r,m+r}}$$

Below is a script file (as it should be typed for use in MatLab) to find the square root of a matrix using Schur decomposition:

```
n=input ('Enter size of a matrix: ')
A=input ('Enter n x n matrix:')
a=A+0.000001i*norm(A)*eye(n,n);
eigvala=eig(a)
[q,t]=schur(a);
b=zeros(n,n);
for m = 1:n
b(m,m)= sqrt(t(m,m));
end;
for m=1:n-1
b(m,m+1)=t(m,m+1)/(b(m,m)+b(m+1,m+1));
end;
for r=2:n-1
for m=1:n-r
B=0;
for k=(m+1):(m+r-1)
B=B+b(m,k)*b(k,m+r);
end;
b(m,m+r)=(t(m,m+r)-B)/(b(m,m)+b(m+r,m+r));
end;
```

end;

b

c=q*b*q'

eigvalc=eig(c)

csquare=c*c

A

er=norm(A-c*c)/norm(A)

Explanation of the Program

n=input ('Enter size of a matrix: '): Indicate the size of the matrix

A=input ('Enter n x n matrix:'): Enter the entries of the matrix enclosed in brackets. Separate each entry with a comma and each row with a semicolon.

a=A+0.000001i*norm(A)*eye(n,n);: If a matrix A is real with complex conjugate eigenvalues, MatLab will automatically return a real matrix with Jordan blocks instead of an upper triangular complex matrix unless we indicate that we are interested in the complex triangular matrix. It is more difficult to compute the square root of a real matrix with Jordan blocks than it is of a triangular one. The term 'eye' in our command refers to the identity matrix, I. The addition, $A + \epsilon I = qtq' + \ \epsilon\ qIq' = q(t + \epsilon I)q'$, will change the matrix t by ϵI, which is very small for small number ϵ. Our computation will show that our results has error less than ϵ.

eigvala=eig(a): This command yields the eigenvalues of the matrix A.

[q,t]=schur(a);: This command shows the breakdown of the matrix A using Schur decomposition. Here q is unitary and t is upper triangular.

b=zeros(n,n);: This command sets all entries of the triangular matrix b to zero to begin the cycle.

```
for m = 1:n
b(m,m)=sqrt(t(m,m));
```

end;: This cycle yields the main diagonal entries for the matrix b.

```
for m=1:n-1
b(m,m+1)=t(m,m+1)/(b(m,m)+b(m+1,m+1));
```

end;: This cycle yields the other diagonal entries $\{b_{12}, b_{23}, b_{34}\}$ for the matrix b.

The following section of the program yields the general formula for finding the matrix entries of b:

$$b_{m,m+r} = \frac{t_{m,m+r} - \sum_{k=m+1}^{m+r+1} b_{m,k} \cdot b_{k,m+r}}{b_{m,m} + b_{m+r,m+r}}, r \geq 2.$$

This formula has two nonnegative terms (or terms with nonnegative real parts) in the denominator. They are square roots of eigenvalues of the given matrix. Even if the given matrix has 2 zero eigenvalues, the denominator will not be zero because of the added matrix 0.000001i*norm(A)*eye(n,n). But in this case the result is not reliable, it may have a larger error.

```
for r=2:n-1
for m=1:n-r
B=0;
for k=(m+1):(m+r-1)
B=B+b(m,k)*b(k,m+r); end;
b(m,m+r)=(t(m,m+r)-B)/(b(m,m)+b(m+r,m+r));
end;
```

end;

b: Prints the matrix b

c=q*b*q': Gives the final result $c = \sqrt{A}$. Since q is a unitary matrix, we can use transpose, q', instead of the inverse, q^{-1} in our program.

eigvalc=eig(c): This command prints the eigenvalues of the matrix c.

csquare=c*c: This command calculates c^2.

A: Prints the matrix A for comparison with matrix c^2.

er=norm(A-c*c)/norm(A): This commands computes the relative error.

Here is an example of computation by the program above:

$\gg$ SchurSqrt(name given to program)

Enter the size of a matrix: 4

Output: n = 4

Enter the matrix $n \times n$: [2, 3, 1, 5; 0, 2, 5, -3; -1, 2, 3, 0; 2, 4, -2, 1]

Output:

$$A = \begin{bmatrix} 2 & 3 & 1 & 5 \\ 0 & 2 & 5 & -3 \\ -1 & 2 & 3 & 0 \\ 2 & 4 & -2 & 1 \end{bmatrix}$$

Output: eigvala=

$$5.1193 + 2.3938i$$

$$5.1193 - 2.3936i$$

$$-1.1193 + 2.3938i$$

$$-1.1193 - 2.3936i$$

Output:

$$q = \begin{bmatrix} -0.3131 + 0.6646i & -0.3443 - 0.3407i & 0.3651 + 0.0808i & -0.1874 - 0.2253i \\ -0.4184 - 0.1222i & -0.3389 + 0.5834i & 0.0488 - 0.3534i & 0.2551 - 0.4030i \\ -0.3214 - 0.0658i & -0.2637 + 0.4194i & -0.0033 + 0.4943i & -0.3791 + 0.5088i \\ -0.1982 + 0.3512i & -0.2096 - 0.1442i & -0.6745 - 0.1832i & 0.3723 + 0.3815i \end{bmatrix}$$

Output:

$$t = \begin{bmatrix} 5.1193 + 2.3938i & 2.3321 - 0.4383i & -2.1173 + 1.5117i & -0.3298 - 2.4575i \\ 0 & 5.1193 - 2.3936i & 2.6075 - 1.9311i & 0.8210 + 2.3928i \\ 0 & 0 & -1.1193 + 2.3938i & 0.1782 + 1.6295i \\ 0 & 0 & 0 & -1.1193 - 2.3936i \end{bmatrix}$$

Output:

$$b = \begin{bmatrix} 2.3206 + 0.5158i & 0.5025 - 0.0944i & -0.2775 + 0.7764i & 0.3460 - 0.6983i \\ 0 & 2.3206 - 0.5157i & 0.6106 - 0.7684i & -0.2512 + 0.4469i \\ 0 & 0 & 0.8727 + 1.3715i & 0.1021 + 0.9336i \\ 0 & 0 & 0 & 0.8727 - 1.3714i \end{bmatrix}$$

Output:

$$c = \begin{bmatrix} 1.2751 + 0.0000i & 0.0942 + 0.0000i & 0.9015 - 0.0000i & 1.7204 - 0.0000i \\ 0.2889 - 0.0000i & 1.7738 + 0.0000i & 0.9570 + 0.0000i & -1.1722 + 0.0000i \\ -0.4103 + 0.0000i & 0.4295 + 0.0000i & 1.8323 + 0.0000i & 0.3623 - 0.0000i \\ 0.4166 + 0.0000i & 1.3518 - 0.0000i & -1.0993 + 0.0000i & 1.5054 + 0.0000i \end{bmatrix}$$

Output: eigvalc=

$$0.8727 + 1.3715i$$

$$0.8727 - 1.3714i$$

$$2.3206 + 0.5158i$$

$$2.3206 - 0.5157i$$

Output: (csquare)

$$c^2 = \begin{bmatrix} 2 & 3 & 1 & 5 \\ 0 & 2 & 5 & -3 \\ -1 & 2 & 3 & 0 \\ 2 & 4 & -2 & 1 \end{bmatrix}$$

Output:

$$A = \begin{bmatrix} 2 & 3 & 1 & 5 \\ 0 & 2 & 5 & -3 \\ -1 & 2 & 3 & 0 \\ 2 & 4 & -2 & 1 \end{bmatrix}$$

Output: er $= 1.0000e - 006$

Once again, to find a matrix $c^2 = A$ using Schur decomposition, we begin with

$$A = qtq^{-1},$$

where q is a unitary matrix and t is an upper triagular matrix. From here we have,

$$b^2 = t,$$

$$b = \sqrt{t},$$

where $\sqrt{t}$ is the principal square root and $c = qbq^{-1}$.

References

[1] S. Athloen and R. McLaughlin, *Gauss-Jordan Reduction: A Brief History*, American Mathematical Monthly 94, 130-142, 1987.

[2] A. Choudhry, *Extraction of nth Roots of* 2×2 *Matrices*, Linear Algebra and its Applications, 387:183-192, 2004.

[3] G.W. Cross, P. Lancaster, Square roots of Complex Matrices, *Linear and Multilinear Algebra*, 289-293, 1974.

[4] L.A. Hageman, D. M. Young, *Applied Iterative Methods*, Academic Press, New York, 1981.

[5] N.J. Higham, *Computing Real Square Roots of a Real Matrix*, Linear Algebra and its Applications, 88/89:405-430, 1987.

[6] N.J. Higham, *Functions of Matrices*, Chapter 11 in Handbook of Linear Algebra, Chapman/CRC Press, Boca Raton, 2007.

[7] N.J. Higham, *Stable Iterations for the Matrix Square Root*, Numerical Algorithms 15, 227-242, 1997.

[8] R.A. Horn, C.R. Johnson, *Matrix Analysis*, Cambridge University Press, 1985.

[9] R.A. Horn, C.R. Johnson, *Topics in Matrix Analysis*, Cambridge University Press, 1991.

[10] T.R. Hughes, I.Levit, and J.Winget, *Element-by-Element Implicit Algorithms for Heat Conduction*, J. Eng. Mech., 109(2), 576-585, 1983.

[11] C.R. Johnson, K. Okubo, and R. Reams, *Uniqueness of Matrix Square Roots and an Application*, Linear Algebra and its Applications, 323:51-60, 2001.

[12] P. Lancaster, M. Tismenetsky, *The Theory of Matrices Second Edition with Applications*, Academic Press, 1985.

[13] D.C. Lay, *Linear Algebra and Its Applications-3rd edition*, Pearson Education, Inc., 2003.

[14] S.J. Leon, *Linear Algebra with Applications-6th edition*, Prentice-Hall,Inc., 2002.

[15] B.W. Levinger, *The Square Root of a* 2×2 *Matrix*, Mathematics Magazine, Vol 53, No.4, 1980.

[16] P.N. Parlett, *The Symmetric Eigenvalue Problem*, Prentice-Hall, Englewood Cliffs, NJ, 1980.

[17] B.A. Schmitt, *An Algebraic Approximation for the Matrix Exponential in Singularly Perturbed Boundary Value Problems*, SIAM J. Numer. Anal. 27(1), 51-66, 1990.

[18] D. Sullivan, *The Square Root of* 2×2 *Matrices*, Mathematics Magazine, Vol 66, No. 5, 1993.

[19] A. Tucker, *The Growing Importance of Linear Algebra in Undergraduate Mathematics*, The College Mathematics Journal, 24, 3-9, 1993.