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Uniqueness of matrix square roots and an application

Charles R. Johnson^a, Kazuyoshi Okubo^b, Robert Reams^{c,*}

^aDepartment of Mathematics, College of William and Mary, P.O. Box 8795, Williamsburg,
VA 23187-8795, USA

^bMathematics Laboratory, Hokkaido University of Education Sapporo, Sapporo 002-8502, Japan

^cDepartment of Mathematics, University of Wyoming, P.O. Box 3036, Laramie, WY 82071-3036, USA

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Abstract

Let $A \in M_n(\mathbb{C})$. Let $\sigma(A)$ denote the spectrum of A , and $F(A)$ the field of values of A . It is shown that if $\sigma(A) \cap (-\infty, 0] = \emptyset$, then A has a unique square root $B \in M_n(\mathbb{C})$ with $\sigma(B)$ in the open right (complex) half plane. This result and Lyapunov's theorem are then applied to prove that if $F(A) \cap (-\infty, 0] = \emptyset$, then A has a unique square root with positive definite Hermitian part. We will also answer affirmatively an open question about the existence of a real square root $B \in M_n(\mathbb{R})$ for $A \in M_n(\mathbb{R})$ with $F(A) \cap (-\infty, 0] = \emptyset$, where the field of values of B is in the open right half plane. © 2001 Elsevier Science Inc. All rights reserved.

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1. Introduction

If $A \in M_n(\mathbb{C})$ has a square root (conditions for this are given in [5, Theorem 6.4.12]), typically it will have many square roots. However, if mild spectral conditions are placed upon the square root, there will often be a “natural” unique one. For

* Corresponding author. Present address: Department of Mathematics, National University of Ireland, Galway, Ireland.

E-mail addresses: crjohnso@math.wm.edu (C.R. Johnson), okubo@atson.sap.hokkyodai.ac.jp (K. Okubo), reams@uwyo.edu (R. Reams).

example, it is well known (and quite useful) that a positive (semi-) definite matrix has a unique positive (semi-) definite square root [4, Theorem 7.2.6], and that this classical fact may be extended to matrices with real and positive spectrum having a unique square root of the same type [5, pp. 287, 488]. Typically, this natural square root may be given via spectral methods, convergent power series, or an integral representation. Our purpose here is to present greatly simplified proofs, extend known uniqueness statements, and to show that the extensions can be applied to answer an open question. When a matrix in a given class \mathcal{C} always has a square root in \mathcal{C} , it is an interesting issue to understand for which \mathcal{C} a uniqueness statement also holds. Our results will be of this type.

We denote by $\sigma(A)$ the set of eigenvalues of $A \in M_n(\mathbb{C})$ (where we agree to list all eigenvalues in the set, including repetitions, e.g. if I is the 3×3 identity matrix we will write $\sigma(I) = \{1, 1, 1\}$). By RHP, we mean the open right half of the complex plane and by $\overline{\text{RHP}}$ its closure (imaginary axis included). The Hermitian part of $A \in M_n(\mathbb{C})$ is $H(A) = \frac{1}{2}(A + A^*)$. The (classical) field of values of $A \in M_n(\mathbb{C})$ is defined by $F(A) = \{x^*Ax : x^*x = 1, x \in \mathbb{C}^n\}$. It is easy to show that A has positive (semi-) definite Hermitian part if and only if $F(A) \subset \text{RHP}$ ($\overline{\text{RHP}}$). Other general properties of $F(A)$, such as compactness and convexity [5, Theorem 1.4.2], are discussed in [5].

It is known [2] that if $A \in M_n(\mathbb{C})$ and $\sigma(A) \subset \text{RHP}$ (or more generally, $\sigma(A) \cap (-\infty, 0] = \emptyset$), then there is a square root of A , $A^{1/2}$ such that $\sigma(A^{1/2}) \subset \text{RHP}$. The region RHP may not be replaced by $\overline{\text{RHP}}$ in this statement without additional knowledge about the Jordan canonical form of A , because some singular matrices have no square roots. Similarly, it is known [7,8] that if $A \in M_n(\mathbb{C})$ and $H(A)$ is positive definite (or more generally, $F(A) \cap (-\infty, 0] = \emptyset$), then there is a square root of A , $A^{1/2}$ such that $H(A^{1/2})$ is positive definite. There are uniqueness statements to go along with both the spectral and field of value facts just mentioned. We provide simplified proofs of these results.

In [6] the question is mentioned and left open as to whether $A \in M_n(\mathbb{R})$, such that $H(A)$ is positive definite, has a square root $A^{1/2} \in M_n(\mathbb{R})$ such that $H(A^{1/2})$ is positive definite. We will show that the answer to this question is in the affirmative.

2. Preliminaries

Lemma 1 extends a result in [9, p. 254]. This extended result for three block matrices A , B and C has a further obvious extension to block tridiagonal matrices with multiple blocks in the appropriate form. We will use e_i to denote the vector with a one in the i th position and zeroes elsewhere.

Lemma 1. *Let $A \in M_l(\mathbb{C})$, $B \in M_m(\mathbb{C})$, $C \in M_n(\mathbb{C})$ and $\sigma(A) = \{\alpha_1, \alpha_2, \dots, \alpha_l\}$, $\sigma(B) = \{\beta_1, \beta_2, \dots, \beta_m\}$ and $\sigma(C) = \{\gamma_1, \gamma_2, \dots, \gamma_n\}$. Define a , b , b_m and c to be eigenvectors as follows:*

$$Aa = \alpha_1 a, \quad Bb_1 = \beta_1 b_1, \quad b_m^* B = \beta_m b_m^*, \quad c^* C = \gamma_n c^*$$

and let $y \in \mathbb{C}^l$, $x, z \in \mathbb{C}^m$, $w \in \mathbb{C}^n$. Then the matrix

$$D = \begin{bmatrix} A & ax^* & 0 \\ b_1 y^* & B & zc^* \\ 0 & w b_m^* & C \end{bmatrix}$$

has eigenvalues $\alpha_2, \alpha_3, \dots, \alpha_l, \beta_2, \beta_3, \dots, \beta_{m-1}, \gamma_1, \gamma_2, \dots, \gamma_{n-1}$, together with the two eigenvalues of

$$\begin{bmatrix} \alpha_1 & x^* b_1 \\ y^* a & \beta_1 \end{bmatrix}$$

and the two eigenvalues of

$$\begin{bmatrix} \beta_m & b_m^* z \\ c^* w & \gamma_n \end{bmatrix}.$$

Proof. There are unitary matrices $U \in M_l(\mathbb{C})$, $V \in M_m(\mathbb{C})$, $W \in M_n(\mathbb{C})$ such that

$$U^* A U = \begin{bmatrix} \alpha_l & \cdots & 0 \\ * & \ddots & \vdots \\ * & * & \alpha_1 \end{bmatrix}, \quad W^* C W = \begin{bmatrix} \gamma_n & \cdots & 0 \\ * & \ddots & \vdots \\ * & * & \gamma_1 \end{bmatrix},$$

where

$$U e_l = \frac{a}{\|a\|}, \quad W e_1 = \frac{c}{\|c\|} \quad \text{and} \quad V^* B V = \begin{bmatrix} \beta_1 & * & * \\ \vdots & \ddots & * \\ 0 & \cdots & \beta_m \end{bmatrix},$$

where

$$V e_1 = \frac{b_1}{\|b_1\|} \quad \text{and} \quad V e_m = \frac{b_m}{\|b_m\|}.$$

Then we have

$$\begin{aligned} & \begin{bmatrix} U^* & 0 & 0 \\ 0 & V^* & 0 \\ 0 & 0 & W^* \end{bmatrix} \begin{bmatrix} A & ax^* & 0 \\ b_1 y^* & B & zc^* \\ 0 & w b_m^* & C \end{bmatrix} \begin{bmatrix} U & 0 & 0 \\ 0 & V & 0 \\ 0 & 0 & W \end{bmatrix} \\ &= \begin{bmatrix} U^* A U & U^* a x^* V & 0 \\ V^* b_1 y^* U & V^* B V & V^* z c^* W \\ 0 & W^* w b_m^* V & W^* C W \end{bmatrix} \end{aligned}$$

Henceforth for $a \notin (-\infty, 0]$, we define \sqrt{a} to be the (unique) square root of a that lies in RHP. Then using Corollary 3, we prove the following:

Lemma 4. *If $A \in M_n(\mathbb{C})$ is an upper triangular matrix such that $\sigma(A) \cap (-\infty, 0] = \emptyset$, then there is a unique matrix B such that $B^2 = A$ and $\sigma(B) \subset \text{RHP}$. Moreover, this matrix B is upper triangular.*

Proof. Let

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & \cdots & a_{1n} \\ 0 & a_{22} & a_{23} & \cdots & a_{2n} \\ \vdots & \cdots & \ddots & \cdots & \vdots \\ \vdots & \cdots & 0 & a_{n-1n-1} & a_{n-1n} \\ 0 & \cdots & \cdots & 0 & a_{nn} \end{bmatrix},$$

where $a_{ii} \notin (-\infty, 0]$ for $1 \leq i \leq n$. By induction on n we demonstrate the uniqueness and upper triangular part of the claim.

If $n = 1$, then $B = \sqrt{a_{11}}$ is the claimed unique square root of A . Assume, then, that the assertion is correct in the case $n - 1$. Let

$$B = \begin{bmatrix} B_{11} & b_{12} \\ b_{21}^* & b_{22} \end{bmatrix},$$

with $B_{11} \in M_{n-1}(\mathbb{C})$ and set $B^2 = A$. Then

$$B^2 = \begin{bmatrix} B_{11}^2 + b_{12}b_{21}^* & (B_{11} + b_{22}I)b_{12} \\ b_{21}^*(B_{11} + b_{22}I) & b_{21}^*b_{12} + b_{22}^2 \end{bmatrix}.$$

Since $B^2 = A$, $b_{21}^*(B_{11} + b_{22}I) = 0$. If $B_{11} + b_{22}I$ is nonsingular, then $b_{21}^* = 0$. Then,

$$B = \begin{bmatrix} B_{11} & b_{12} \\ 0 & b_{22} \end{bmatrix}.$$

Now $b_{22} = \sqrt{a_{nn}}$, and with the inductive assumption that B_{11} is the unique square root of A_{11} (the upper left $(n - 1) \times (n - 1)$ principal submatrix of A) with $\sigma(B_{11}) \subset \text{RHP}$ and B_{11} upper triangular, it is easy to calculate b_{12} and thus B is uniquely determined. If $B_{11} + b_{22}I$ were singular and $b_{21} \neq 0$, then $-b_{22}$ would be an eigenvalue of B_{11} (and b_{21} would be a corresponding left eigenvector). By Corollary 3, however, the eigenvalues of B would then be those of B_{11} , besides $-b_{22}$, together with the two eigenvalues of

$$X = \begin{bmatrix} -b_{22} & b_{21}^*b_{12} \\ 1 & b_{22} \end{bmatrix}.$$

However, since $\text{trace}(X) = 0$, the requirement that $\sigma(B) \subset \text{RHP}$ would then be contradicted.

It remains only to ensure the existence of any square root B of A with the given hypotheses on A , and with $\sigma(B) \subset \text{RHP}$. This can be done most easily as in [1]

by letting B be an upper triangular matrix, setting $B^2 = A$, and observing that it is possible to solve for B , starting with the main diagonal and then solving for each superdiagonal successively. Thus

$$b_{ii} = \sqrt{a_{ii}}, \quad b_{ij} = \frac{1}{\sqrt{a_{ii}} + \sqrt{a_{jj}}} \left[a_{ij} - \sum_{k=i+1}^{j-1} b_{ik}b_{kj} \right], \quad i < j,$$

and since $a_{ii} \notin (-\infty, 0]$ then $\sqrt{a_{ii}}$ is in RHP for each i . \square

Remarks. There may be square roots of an upper triangular matrix that are not upper triangular (as discussed in [1]), for example,

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

Lemma 4 states that the square root matrix B must be upper triangular, with the given hypotheses on A , and when we require $\sigma(B) \subset \text{RHP}$, which is not evident from [2]. The procedure described in [1] was primarily intended for matrices with real entries, for which we included the details since we modify their procedure below. Theorem 5 below can also be obtained from the theory of Jordan Form and primary matrix functions in the way outlined in [5, pp. 287, 488], where the spectrum of their A is real and positive. We note that our proofs are quite different.

3. Results with simplified proofs

Theorem 5 is a natural consequence of Lemma 4, and we will use it to prove Theorem 7.

Theorem 5. *Let $A \in M_n(\mathbb{C})$ be such that $\sigma(A) \cap (-\infty, 0] = \emptyset$. Then there is a unique $B \in M_n(\mathbb{C})$ such that $B^2 = A$ with $\sigma(B) \subset \text{RHP}$.*

Proof. Let λ_i ($i = 1, 2, \dots, n$) be the eigenvalues of A . From Schur's theorem, there is a unitary matrix U such that

$$A = U^* \begin{bmatrix} \lambda_1 & a_{12} & \cdots & a_{1n} \\ 0 & \lambda_2 & \cdots & \vdots \\ \vdots & \cdots & \ddots & a_{n-1n} \\ 0 & \cdots & 0 & \lambda_n \end{bmatrix} U = U^* A' U.$$

Then from Lemma 4, there is a unique upper triangular matrix C such that $C^2 = A'$ and $\sigma(C) \subset \text{RHP}$. We can take $B = U^* C U$. Now if $B, B' \in M_n$ satisfy $B^2 = B'^2 = A$ and $\sigma(B), \sigma(B') \subset \text{RHP}$, then

$$\begin{bmatrix} \lambda_1 & a_{12} & \cdots & a_{1n} \\ 0 & \lambda_2 & \cdots & \vdots \\ \vdots & \cdots & \ddots & a_{n-1n} \\ 0 & \cdots & 0 & \lambda_n \end{bmatrix} = UAU^* = (UBU^*)^2 = (UB'U^*)^2.$$

The uniqueness in Lemma 4 gives $UBU^* = UB'U^*$, which implies $B = B'$. \square

Corollary 6. *Let $A \in M_n(\mathbb{R})$ be such that $\sigma(A) \cap (-\infty, 0] = \emptyset$. Then there is a unique $B \in M_n(\mathbb{R})$ such that $B^2 = A$ with $\sigma(B) \subset \text{RHP}$.*

Proof. If we show that for $A \in M_n(\mathbb{R})$ there exists $B \in M_n(\mathbb{R})$ with $B^2 = A$ and $\sigma(B) \subset \text{RHP}$, then the uniqueness follows from the uniqueness of Theorem 5.

We first perform a similarity on A with $S \in M_n(\mathbb{R})$, so that $S^{-1}AS$ is in upper Hessenberg form with 1×1 blocks or 2×2 blocks of form

$$\begin{bmatrix} a & b \\ -b & a \end{bmatrix} \in M_2(\mathbb{R})$$

down the diagonal. Using the real Jordan form described in [4, Theorem 3.4.5], we know that we can perform this similarity, and we shall arrange for all of these 2×2 diagonal blocks to be placed adjacent to each other down the diagonal starting from the top left corner, so that thereafter all 1×1 diagonal blocks are placed adjacent to each other down to the bottom right corner.

To find a square root B for $S^{-1}AS$ we modify the procedure of Björck and Hammarling [1]. B will be an upper Hessenberg matrix with an entry below the diagonal when there is a 2×2 block of form

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

on the diagonal of $S^{-1}AS$. Thus, if (say) one of these 2×2 blocks is in the top left corner of $S^{-1}AS$, then take

$$b_{12} = \sqrt{\frac{-a + \sqrt{a^2 + b^2}}{2}} = -b_{21},$$

solve for b_{11} in the equation $b_{11}b_{12} = b/2$, and set $b_{22} = b_{11}$. Continue in this way determining all 2×2 and 1×1 blocks down the diagonal of B (the 1×1 blocks are determined as previously described). If n is even, now, take all 1×1 blocks in pairs to form 2×2 blocks where the bottom left entry of each 2×2 block is 0, and the top right entry determined as previously described. If n is odd, take all 1×1 blocks in pairs, except that the very bottom right entry of $S^{-1}AS$ is left unpaired, and will be dealt with as described below. Suppose again now that n is even and consider B as having its top two rows consisting of the 2×2 blocks $B_{11}, B_{12}, B_{13}, \dots, B_{1m}$, where $n = 2m$. Then B_{12} can be solved for in the equation $B_{11}B_{12} + B_{12}B_{22} = A_{12}$ (where $S^{-1}AS = (A_{ij})$ is written as a matrix of 2×2 blocks) in the usual way using

Kronecker products [5, Theorem 4.4.6], since B_{ii} has its eigenvalues in RHP for each i , $1 \leq i \leq m$. Proceeding in this way we can determine all 2×2 blocks B_{ii+1} down the (block) superdiagonal adjacent to the main diagonal. Thus, we are performing a 2×2 block version of Björck and Hammerling's [1] method. Continue in this way for all 2×2 blocks in B solving for each (block) superdiagonal successively. If n is odd, where $n = 2m + 1$, proceed exactly as above when n is even, with the top left $(n - 1) \times (n - 1)$ block of B as a matrix of 2×2 blocks. The last column is determined by taking $B_{i(m+1)}$ as a column vector in \mathbb{R}^2 , for each i , $1 \leq i \leq m$. Moreover, take $B_{(m+1)(m+1)} = b_{nn}$ as an element of \mathbb{R} , and in this case $B_{ii} + b_{nn}I$ is invertible. Again, each superdiagonal can be solved for successively. \square

For a comparison of stable algorithms to compute matrix square roots see [3]. In the above algorithm all 2×2 blocks of B may be solved for explicitly in terms of entries if desired.

We note that both existence and uniqueness fail if $\sigma(A) \cap (-\infty, 0] = \emptyset$ is replaced by $\sigma(A) \cap (-\infty, 0) = \emptyset$ in the statement of Theorem 5. For example,

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

has no square root and

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

has the family of square roots

$$\begin{bmatrix} 0 & x & 0 \\ 0 & 0 & 1/x \\ 0 & 0 & 0 \end{bmatrix}, \quad x \in \mathbb{C} \setminus \{0\}.$$

In order to prove Theorem 7, we will use Lyapunov's theorem which is most commonly stated with $A \in M_n(\mathbb{C})$ positive stable, that is, each eigenvalue of A is in RHP.

Lyapunov's theorem. *Let $A \in M_n(\mathbb{C})$ be positive stable. If $AX + XA^*$ is positive definite, then X is positive definite, where $X \in M_n(\mathbb{C})$.*

Although a more general form of Lyapunov's theorem is given in [5, Theorem 2.2.1], the above version is all we need. Let us call the “ $(\pi/4)$ -cone” that wedge-shaped region of the complex plane bounded by the lines $y = \pm x$, more precisely given by $\{z \in \mathbb{C} \setminus \{0\} \mid \text{Arg}(z) < \pi/4\}$.

Theorem 7 [7,8]. *If $A \in M_n(\mathbb{C})$ is such that $F(A) \cap (-\infty, 0] = \emptyset$, then there is a unique $B \in M_n(\mathbb{C})$ such that $B^2 = A$ and $F(B) \subset \text{RHP}$. Moreover, if $\text{Im}(A) =$*

$(A - A^*)/2i$ is positive definite, then $\text{Im}(B)$ is positive definite, while if $\text{Im}(A)$ is negative definite, then $\text{Im}(B)$ is negative definite.

Proof. Since $F(A) \cap (-\infty, 0] = \emptyset$, there is θ such that $|\theta| < \pi/2$ and $F(e^{i\theta}A) \subset \text{RHP}$ [5, proof of Theorem 1.3.5]. Put $C = e^{i\theta}A$, so C has positive definite Hermitian part and $\sigma(C) \subset \text{RHP}$. From Theorem 5 there is a unique $D \in M_n(\mathbb{C})$ such that $D^2 = C$ with $\sigma(D) \subset \text{RHP}$.

Write

$$D(D + D^*) + (D + D^*)D^* = D^2 + D^{*2} + 2DD^* = C + C^* + 2DD^*.$$

Since $C + C^*$ is positive definite and D is positive stable, Lyapunov’s theorem implies that $D + D^*$ is positive definite. Let $B = e^{-i\theta/2}D$. Then $B^2 = e^{-i\theta}D^2 = e^{-i\theta}C = A$. We claim that $B + B^*$ is positive definite. We have just shown that $e^{i\theta/2}B + e^{-i\theta/2}B^*$ is positive definite, that is $F(e^{i\theta/2}B) \subset \text{RHP}$, so that $F(B) \subset e^{-i\theta/2}(\text{RHP})$. Now, let $\lambda \in \sigma(B)$, then $\lambda^2 \in \sigma(A)$ and $e^{i\theta}\lambda^2 \in \sigma(e^{i\theta}A) \subset F(e^{i\theta}A) \subset \text{RHP}$. So $e^{i\theta}\lambda^2 \in \text{RHP}$ and $\pm e^{i\theta/2}\lambda \in (\pi/4)$ -cone. But $\pm\lambda \in e^{-i\theta/2}(\pi/4)$ -cone $\subset e^{-i\theta/2}\text{RHP}$ implies $\lambda \in e^{-i\theta/2}(\pi/4)$ -cone, and so $e^{i\theta}\lambda \in e^{i\theta/2}(\pi/4)$ -cone $\subset \text{RHP}$, since $-\pi/4 < \theta/2 < \pi/4$. Thus $e^{i\theta}B$ is positive stable. Then consider

$$e^{i\theta}B(B + B^*) + (B + B^*)e^{-i\theta}B^* = e^{i\theta}B^2 + e^{-i\theta}B^{*2} + (e^{i\theta} + e^{-i\theta})BB^*.$$

Since $e^{i\theta} + e^{-i\theta} = 2\cos\theta$ and $-\pi/2 < \theta < \pi/2$, we know $e^{i\theta} + e^{-i\theta} > 0$, and because $e^{i\theta}A + e^{-i\theta}A^*$ is positive definite, we can conclude that $B + B^*$ is positive definite as before.

The uniqueness of B follows as a special case of Theorem 5.

For the last part of the theorem, suppose that $\text{Im}(A)$ is positive definite and consider

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

Since $\text{Im}(A)$ is positive definite and B is positive stable, so Lyapunov’s theorem tells us that $\text{Im}(B)$ is positive definite. Similarly, $\text{Im}(A)$ negative definite implies that $\text{Im}(B)$ is negative definite. \square

4. Answer to an open question

In [6] the following question was mentioned but left unanswered: Suppose that $A \in M_n(\mathbb{R})$ satisfies $F(A) \cap (-\infty, 0] = \emptyset$. Does A then have a square root $A^{1/2} \in M_n(\mathbb{R})$ such that $F(A^{1/2}) \subset \text{RHP}$? (It was, of course, known that it had a complex such square root.) Our considerations allow us to answer this question.

Corollary 8. *If $A \in M_n(\mathbb{R})$ is such that $F(A) \cap (-\infty, 0] = \emptyset$, then there is a unique $B \in M_n(\mathbb{R})$ such that $B^2 = A$ and $F(B) \subset \text{RHP}$.*

Proof. Since $\sigma(A) \cap (-\infty, 0] = \emptyset$, we know from Corollary 6 that there is a unique $B \in M_n(\mathbb{R})$ such that $B^2 = A$, with $\sigma(B) \subset \text{RHP}$. We saw in the proof of Theorem 7 that A has a unique square root B' such that $F(B') \subset \text{RHP}$. But then $\sigma(B') \subset \text{RHP}$, so we must have $B = B'$. Hence the question is answered affirmatively. \square

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