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Square Roots of Real 3×3 Matrices vs. Quartic Polynomials with Real Zeros

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Abstract

There is an interesting analogy between the description of the real square roots of 3×3 matrices and the zeros of the (depressed) real quartic polynomials. This analogy, which in fact better explains the nature of the zeros of those polynomials, is unveiled through a natural use of the Cayley-Hamilton theorem.

1. Introduction

Only non-negative real numbers admit real square roots. Thinking of a real number as the simplest square matrix, a 1×1 matrix, an interesting question emerges: Which real $n \times n$ matrices, $n \geq 1$, admit real square roots? In other words, for which $A \in \mathrm{Mat}(n, n, \mathbf{R}) := \mathrm{Mat}(n, \mathbf{R})$ is there an $S \in \mathrm{Mat}(n, \mathbf{R})$ such that $S^2 = A$?

It should not be a complete surprise that an answer to this question might have unexpected consequences. After all, the simplest case, $n = 1$, leads to the concept of complex number! In the same vain we want to show now that the case $n = 3$ is equivalent to understanding (and in fact better explains) the nature of the zeros of the (depressed) quartic polynomials in indeterminate λ, $\lambda^4 + q\lambda^2 + r\lambda + s$, $q, r, s \in \mathbf{R}$.

The study of square roots of matrices, either complex or real, has a long history. It was initiated by Cayley [3, 4], who treated the cases $n = 2, 3$, and was continued by Taber [15], Metzler [10], Frobenius [6], Baker [2], and many others (For a detailed account, see [7, 8]). In fact, an answer in the general case exists [5, 7, 8]:

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Theorem 0. *For a matrix $A \in \mathrm{Mat}(n, \mathbf{R})$ there is an $S \in \mathrm{Mat}(n, \mathbf{R})$ such that $S^2 = A$ if and only if in the sequence of integers $d_1, d_2, \ldots, d_i := \dim\ker(A^i) - \dim\ker(A^{i-1})$, no two consecutive terms are the same odd integer, and A has an even number of Jordan blocks of each size for every negative eigenvalue.*

For arbitrary n, clearly $\det A \geq 0$ is a necessary condition for the existence of real square roots, since $A = S^2$ implies $\det A = \det^2 S \geq 0$. If A is a positive diagonal matrix, $A = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, $\lambda_1, \lambda_2, \ldots, \lambda_n \geq 0$, then $S = \mathrm{diag}(\pm\sqrt{\lambda_1}, \pm\sqrt{\lambda_2}, \ldots, \pm\sqrt{\lambda_n})$ provide up to 2^n real square roots for A. This might suggest that subjecting A first to some canonical form, such as the Jordan canonical form, could be a way of reducing the original problem to a simpler one, which is also the approach taken for deriving Theorem 0.

Another way, we judge better for small size matrices, is in the spirit of the pioneering work of Cayley and makes use of the characteristic polynomial of A, $\chi_A(\lambda) := \det(\lambda I - A)$, where, as usual, I is the identity $n \times n$ matrix. It is possible to conclude this way that the real square roots of A effectively depend on the existence of real zeros for a suitable polynomial of degree 2^n, which can be replaced by a degree 2^{n-1} one for n odd.

The case $n = 2$ has already been worked out in every detail by this method, in three seemingly unrelated papers [1, 9, 14], even if [9, 14] deal mainly with complex matrices. It turns out [1] that $A \in \mathrm{Mat}(2, \mathbf{R})$ admits real square roots if and only if $\det A \geq 0$ and either $\mathrm{tr}\, A + 2\sqrt{\det A} > 0$ or else $A = -\sqrt{\det A} I$. In fact, there are two or four possible square roots for A if the minimal polynomial of A has degree 2, and infinitely many, if it has degree 1, i. e., $A = aI$, $a \in \mathbf{R}$.

While the method outlined below works in principle for arbitrary $n \times n$ matrices only the small n cases ($n = 2, 3$) produce compelling results. We therefore dedicate the rest of the paper to the case $n = 3$.

2. Square Roots of Real 3 × 3 Matrices – Part I

For any 3×3 real matrix M, its characteristic polynomial $\chi_M(\lambda)$ is

$$\chi_M(\lambda) = \det(\lambda I - M) = \lambda^3 - (\mathrm{tr}\, M)\lambda^2 + (\mathrm{ch}\, M)\lambda - \det M. \tag{1}$$

tr, ch, and det above are similarity invariants of a 3×3 matrix, the familiar trace and determinant, while ch is the sum of the three (unsigned) diagonal minors obtained by deleting the same row and column from the matrix. Famously (Cayley-Hamilton theorem), each matrix is a root of its characteristic polynomial, i. e.,

$$M^3 - (\mathrm{tr}\, M)M^2 + (\mathrm{ch}\, M)M - (\det M)I = 0. \tag{2}$$

Assume now that a real 3×3 matrix A admits a real square root S. Since $S^2 = A$, equation (2) applied to S gives

$$AS - (\mathrm{tr}\, S)A + (\mathrm{ch}\, S)S - (\det S)I = 0. \tag{3}$$

Multiplying (3) by S yields

$$A^2 - (\operatorname{tr} S)AS + (\operatorname{ch} S)A - (\det S)S = 0. \tag{4}$$

Finally, replacing in (4) AS by its expression as a linear combination of A, S, and I given by (3), allows one to write

$$((\operatorname{tr} S)(\operatorname{ch} S) - \det S)S = -A^2 + (\operatorname{tr}^2 S - \operatorname{ch} S)A + (\operatorname{tr} S)(\det S)I. \tag{5}$$

There is an obvious way to relate the characteristic invariants of S and A. It comes from

$$\det(\lambda^2 I - A) = \det(\lambda I - S)(\lambda I + S) = \det(\lambda I - S)\det(\lambda I + S). \tag{6}$$

Via (1), (6) is now equivalent to

$$\begin{aligned} &\lambda^6 - (\operatorname{tr} A)\lambda^4 + (\operatorname{ch} A)\lambda^2 - \det A = \\ &(\lambda^3 - (\operatorname{tr} S)\lambda^2 + (\operatorname{ch} S)\lambda - \det S)(\lambda^3 + (\operatorname{tr} S)\lambda^2 + (\operatorname{ch} S)\lambda + \det S). \end{aligned} \tag{7}$$

By identifying the coefficients of λ in (7) we get

$$\begin{aligned} \operatorname{tr} A &= \operatorname{tr}^2 S - 2\operatorname{ch} S \\ \operatorname{ch} A &= \operatorname{ch}^2 S - 2(\operatorname{tr} S)(\det S) \\ \det A &= \det^2 S \end{aligned} \tag{8}$$

Since $-S$ is also a square root of A, and for n odd, $\det(-S) = -\det S$, there is no loss of generality in assuming $\det S \geq 0$. The first and last equations in (8) thus become

$$\begin{aligned} \operatorname{ch} S &= \frac{\operatorname{tr}^2 S - \operatorname{tr} A}{2} \\ \det S &= \sqrt{\det A}, \end{aligned} \tag{9}$$

and consequently the second one is equivalent to

$$\operatorname{tr}^4 S - 2(\operatorname{tr} A)\operatorname{tr}^2 S - 8\sqrt{\det A}\operatorname{tr} S + \operatorname{tr}^2 A - 4\operatorname{ch} A = 0. \tag{10}$$

Also, (5) is seen to be equivalent, via (9), to

$$(\operatorname{tr}^3 S - (\operatorname{tr} A)\operatorname{tr} S - 2\sqrt{\det A})S = -2A^2 + (\operatorname{tr}^2 S + \operatorname{tr} A)A + 2\sqrt{\det A}(\operatorname{tr} S)I. \tag{11}$$

We just proved the following

Theorem 1. *If S is a real square root of some matrix $A \in \mathrm{Mat}(3, \mathbf{R})$ such that $\det S \geq 0$, then necessarily $\det A \geq 0$, $\operatorname{tr} S$ must be a (real) zero of the quartic polynomial*

$$p_A(\lambda) := \lambda^4 - 2(\operatorname{tr} A)\lambda^2 - 8\sqrt{\det A}\lambda + \operatorname{tr}^2 A - 4 \operatorname{ch} A, \tag{12}$$

and

$$(p'_A(\operatorname{tr} S)/4)S = -2A^2 + (\operatorname{tr}^2 S + \operatorname{tr} A)A + 2\sqrt{\det A}(\operatorname{tr} S)I. \tag{13}$$

Consequently, (13) expresses S uniquely in terms of A and $\operatorname{tr} S$, if $\operatorname{tr} S$ is a simple real zero of $p_A(\lambda)$.

Conversely, easy calculations show that if $A \in \mathrm{Mat}(3, \mathbf{R})$ has $\det A \geq 0$ and the quartic polynomial $p_A(\lambda)$ admits a simple real zero, say τ, then

$$S := \frac{4}{p'_A(\tau)} \left(-2A^2 + (\tau^2 + \operatorname{tr} A)A + 2\sqrt{\det A}\tau I \right) \tag{14}$$

is a real square root of A. Moreover, $\operatorname{tr} S = \tau$ and $\det S = \sqrt{\det A}$.

3. Nature of the Zeros of a Depressed Real Quartic Polynomial

Theorem 1 puts an interesting twist on a classical problem — the nature (real or complex conjugate, simple or multiple) of the four (complex) zeros of a monic quartic polynomial in λ, $\lambda^4 + p\lambda^3 + q\lambda^2 + r\lambda + s$, as the real coefficients p, q, r and s vary. There are few ways of addressing this problem, or the historically old problem of solving for the actual zeros [11, 12, 13]. They all eventually involve the discriminant quantity

$$\Delta := \prod_{1 \leq i < j \leq 4} (z_i - z_j)^2, \ z_1, \ldots, z_4 \text{ complex zeros of the quartic polynomial.} \tag{15}$$

Δ has two fundamental features: being a symmetric function of the zeros, it is expressible as a (complicated) function of the polynomial coefficients, and its vanishing is an indicator of multiple zeros.

There is one standard way of somewhat simplifying the discriminant Δ, based of the substitution $\lambda \longrightarrow \lambda + p/4$, which reduces the quartic polynomial to a depressed form of type $\lambda^4 + q\lambda^2 + r\lambda + s$. Also, there is no loss of generality in assuming $r \leq 0$, since z is a zero of $\lambda^4 + q\lambda^2 + r\lambda + s$ if and only if $-z$ is a zero of $\lambda^4 + q\lambda^2 - r\lambda + s$.

Theorem 1 may suggest that writing the depressed quartic polynomial as

$$\lambda^4 - 2t\lambda^2 - 8\sqrt{d}\lambda + t^2 - 4c, \quad t, d, c \text{ arbitrary reals}, d \geq 0, \tag{16}$$

could simplify the discriminant Δ, and indeed this is the case. It can be shown based on a general formula for Δ [16] that for the depressed quartic polynomial (16) one has

$$\begin{aligned}\Delta &= -\,2^{12}\left(27d^2 + 2t(2t^2 - 9c)d + c^2(4c - t^2)\right)\\ &= -\,\frac{2^{12}}{3^3}\left(\left(27d + t(2t^2 - 9c)\right)^2 - 4(t^2 - 3c)^3\right).\end{aligned} \tag{17}$$

Most treatments on the nature of the zeros of the depressed quartic polynomial $\lambda^4 + q\lambda^2 + r\lambda + s$ condition first on the sign of Δ, then given Δ on the sign of q, to finish with conditions on s, given Δ and q. To the best of our knowledge only one reference, [11], takes a geometric approach to the problem resulting in conditioning in the order q, then s, then Δ. Interestingly enough, in a footnote to [11], an Editor of the Amer. Math. Monthly, 1922, suggests that one could eventually do away with Δ, and accomplish a more desirable conditioning on r instead.

It turns out that by using the depressed quartic polynomial in the form given by (16) the above suggestion comes to fore in a very economical and esthetically pleasing way, as we shall see below.

Geometrically, the real zeros of the depressed quartic polynomial (16) appear as the abscissas of the intersection points, in a xOy coordinate system, of the even quartic graph $y = (x^2 - t)^2 - 4c$, $t, c \in \mathbf{R}$, and the line $y = 8\sqrt{d}x$, $d \geq 0$. Clearly, the signs of t and c dictate how a variable line through the origin intersects a fixed quartic graph. Moreover, multiple real zeros can occur only at points where the line is tangent to the quartic. They correspond to values of t, s, and d for which Δ vanishes.

The figures below show how variable lines through the origin intersect a fixed quartic graph, for two specific instances of the latter.

Based on the above geometric realization of the real zeros of the depressed quartic polynomial (16) and on the expression of the discriminant given by (17) the following theorem holds true (compare also to [11]).

Theorem 2. *A complete description of the nature of the real zeros of the depressed quartic polynomial* $\lambda^4 - 2t\lambda^2 - 8\sqrt{d}\lambda + t^2 - 4c$, $t, c, d \in \mathbf{R}$, $d \geq 0$ *is as follows:*

Case I. $t > 0$,

$c < 0$,

$0 \leq d < \frac{2(t^2-3c)\sqrt{t^2-3c} - t(2t^2-9c)}{27}$, *no real zeros;*

$d = \frac{2(t^2-3c)\sqrt{t^2-3c} - t(2t^2-9c)}{27}$, *two zeros real and equal;*

$d > \frac{2(t^2-3c)\sqrt{t^2-3c} - t(2t^2-9c)}{27}$, *two zeros real and distinct;*

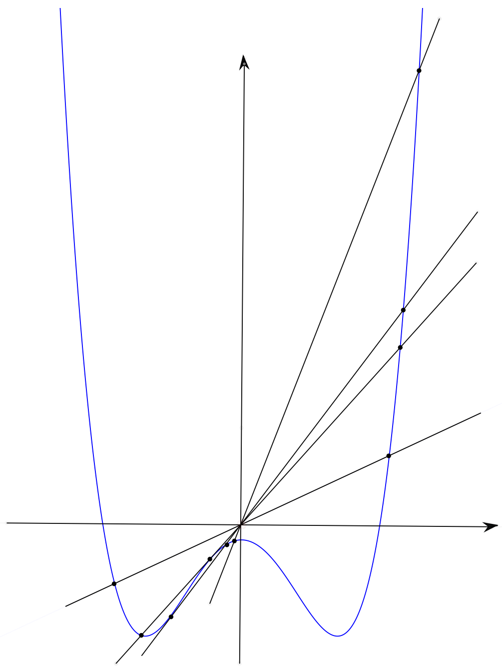

Figure 1: $t > 0$, $t^2/4 < c < t^2/3$

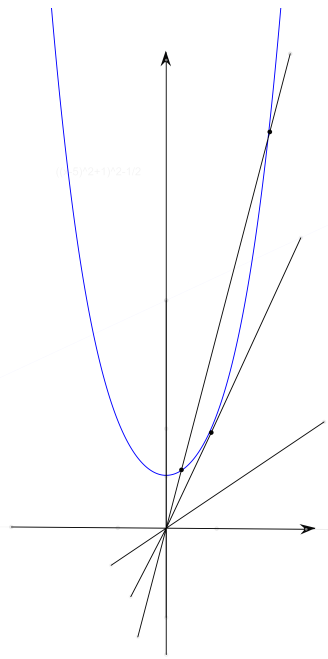

FIGURE 2. $t < 0$, $c < t^2/4$

$c = 0$,

$d = 0$, two pairs of equal real zeros, $-\sqrt{t}, -\sqrt{t}, \sqrt{t}, \sqrt{t}$;

$d > 0$, two zeros real and distinct;

$0 < c < t^2/4$,

$0 \le d < \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, all zeros real and distinct;

$d = \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, all zeros real, two equal;

$d > \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, two zeros real and distinct;

$c = t^2/4$,

$d = 0$, all zeros real, two equal, $-\sqrt{2t}, 0, 0, \sqrt{2t}$;

$0 < d < \frac{t^3}{54}$, all zeros real and distinct;

$d = \frac{t^3}{54}$, all zeros real, two equal;

$d > \frac{t^3}{54}$, two zeros real and distinct;

$t^2/4 < c < t^2/3$,

$0 \le d < \frac{-2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, *two zeros real and distinct;*

$d = \frac{-2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, *all zeros real, two equal;*

$\frac{-2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27} < d < \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, *all zeros real and distinct;*

$d = \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, *all zeros real, two equal;*

$d > \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, *two zeros real and distinct;*

$c = t^2/3$,

$d = \frac{t^3}{27}$, *all zeros real, three equal,* $-\sqrt{\frac{t}{3}}, -\sqrt{\frac{t}{3}}, -\sqrt{\frac{t}{3}}, \sqrt{3t}$;

$d \neq \frac{t^3}{27}$, *two zeros real and distinct;*

$c > t^2/3$;

$d \ge 0$, *two zeros real and distinct;*

Case II. $t = 0$,

$c < 0$,

$0 \le d < -\frac{2c\sqrt{-c}}{3\sqrt{3}}$, *no real zeros;*

$d = -\frac{2c\sqrt{-c}}{3\sqrt{3}}$, *two zeros real and equal,* $\sqrt{2}\sqrt[4]{-\frac{c}{3}}, \sqrt{2}\sqrt[4]{-\frac{c}{3}}$;

$d > -\frac{2c\sqrt{-c}}{3\sqrt{3}}$, *two zeros real and distinct;*

$c = 0$,

$d = 0$, *four equal real zeros,* $0, 0, 0, 0$;

$d > 0$, *two zeros real and distinct,* $0, 2\sqrt[6]{d}$;

$c > 0$,

$d \ge 0$, *two zeros real and distinct;*

Case III. $t < 0$,

$c < t^2/4$,

$0 \le d < \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, *no real zeros;*

$d = \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, *two zeros real and equal;*

$d > \frac{2(t^2-3c)\sqrt{t^2-3c}-t(2t^2-9c)}{27}$, *two zeros real and distinct;*

$c = t^2/4$,

$d = 0$, *two zeros real and equal, 0, 0;*

$d > 0$, *two zeros real and distinct;*

$c > t^2/4$,

$d \geq 0$, *two zeros real and distinct;*

4. Square Roots of Real 3 × 3 Matrices – Part II

We conclude the paper with a complete, and most importantly very practical, characterization of all 3×3 real matrices which admit real square roots.

It is worth recalling that any monic cubic polynomial $\lambda^3 + p\lambda^2 + q\lambda + r$, $p, q, r \in \mathbf{R}$, is the minimal polynomial of some matrix $A \in \mathrm{Mat}(3, \mathbf{R})$, for instance of $A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -r & -q & -p \end{bmatrix}$. Also, $\lambda^2 + p\lambda + q$, $p, q \in \mathbf{R}$ is the minimal polynomial of some matrix $A \in \mathrm{Mat}(3, \mathbf{R})$ if and only if $p^2 - 4q \geq 0$. To that end, $A = \begin{bmatrix} 0 & 1 & 0 \\ -q & -p & 0 \\ 0 & 0 & r \end{bmatrix}$, r real zero of $\lambda^2 + p\lambda + q$, will do in the $p^2 - 4q \geq 0$ case, while if $p^2 - 4q < 0$ no $A \in \mathrm{Mat}(3, \mathbf{R})$ satisfies $A^2 + pA + qI = 0$, since any 3×3 real matrix admits at least one real eigenvalue. Finally, $A = -pI$, $p \in \mathbf{R}$, has minimal polynomial $\lambda + p$.

In the following corollary vectors in $\mathbf{R}^3$ or $\mathbf{R}^2$ are to be interpreted as column vectors (3×1 or 2×1 matrices), '$(\ )^T$' denotes matrix transposition and '$\cdot$' stands for the Euclidean dot product.

Corollary. *A complete description of the matrices* $A \in \mathrm{Mat}(3, \mathbf{R})$ *with characteristic polynomial* $\chi_A(\lambda) = \lambda^3 - (\mathrm{tr}\, A)\lambda^2 + (\mathrm{ch}\, A)\lambda - \det A$ *which admit real square roots* $S \in \mathrm{Mat}(3, \mathbf{R})$ *is as follows:*

a) If the minimal polynomial of A *equals its characteristic polynomial then* A *admits (finitely many) real square roots if and only if* $\det A \geq 0$ *and* $\mathrm{tr}\, A$, $\mathrm{ch}\, A$, *and* $\det A$ *satisfy one of the following nested systems of inequalities (the number of square roots is indicated in each case):*

$\mathrm{tr}\, A > 0$,

$\mathrm{ch}\, A \leq 0$,

$\det A > \frac{2(\mathrm{tr}^2 A - 3\,\mathrm{ch}\, A)\sqrt{\mathrm{tr}^2 A - 3\,\mathrm{ch}\, A} - \mathrm{tr}\, A(2\,\mathrm{tr}^2 A - 9\,\mathrm{ch}\, A)}{27}$, *four roots;*

$0 < \mathrm{ch}\, A < \mathrm{tr}^2 A/4$,

$0 \leq \det A < \frac{2(\mathrm{tr}^2 A - 3\,\mathrm{ch}\, A)\sqrt{\mathrm{tr}^2 A - 3\,\mathrm{ch}\, A} - \mathrm{tr}\, A(2\,\mathrm{tr}^2 A - 9\,\mathrm{ch}\, A)}{27}$, *eight-roots;*

$\det A \geq \frac{2(\mathrm{tr}^2 A - 3\,\mathrm{ch}\, A)\sqrt{\mathrm{tr}^2 A - 3\,\mathrm{ch}\, A} - \mathrm{tr}\, A(2\,\mathrm{tr}^2 A - 9\,\mathrm{ch}\, A)}{27}$, *four roots;*

$\mathrm{ch}\, A = \mathrm{tr}^2 A/4$,

$\det A = 0$, *four roots;*

$0 < \det A < \frac{\operatorname{tr}^3 A}{54}$, *eight roots;*

$\det A \geq \frac{\operatorname{tr}^3 A}{54}$, *four roots;*

$\operatorname{tr}^2 A/4 < \operatorname{ch} A < \operatorname{tr}^2 A/3$,

$0 \leq \det A \leq \frac{-2(\operatorname{tr}^2 A - 3\operatorname{ch} A)\sqrt{\operatorname{tr}^2 A - 3\operatorname{ch} A} - \operatorname{tr} A(2\operatorname{tr}^2 A - 9\operatorname{ch} A)}{27}$, *four-roots;*

$\left|\det A + \frac{\operatorname{tr} A(2\operatorname{tr}^2 A - 9\operatorname{ch} A)}{27}\right| < \frac{2(\operatorname{tr}^2 A - 3\operatorname{ch} A)\sqrt{\operatorname{tr}^2 A - 3\operatorname{ch} A}}{27}$, *eight-roots;*

$\det A \geq \frac{2(\operatorname{tr}^2 A - 3\operatorname{ch} A)\sqrt{\operatorname{tr}^2 A - 3\operatorname{ch} A} - \operatorname{tr} A(2\operatorname{tr}^2 A - 9\operatorname{ch} A)}{27}$, *four roots;*

$\operatorname{ch} A = \operatorname{tr}^2 A/3$,

$\det A = \frac{\operatorname{tr}^3 A}{27}$, *two roots;*

$\det A \neq \frac{\operatorname{tr}^3 A}{27}$, *four roots;*

$\operatorname{ch} A > \operatorname{tr}^2 A/3$;

$\det A \geq 0$, *four roots;*

$\operatorname{tr} A = 0$,

$\operatorname{ch} A \leq 0$,

$\det A > -\frac{2\operatorname{ch} A\sqrt{-\operatorname{ch} A}}{3\sqrt{3}}$, *four roots;*

$\operatorname{ch} A > 0$,

$\det A \geq 0$, *four roots;*

$\operatorname{tr} A < 0$,

$\operatorname{ch} A \leq \operatorname{tr}^2 A/4$,

$\det A > \frac{2(\operatorname{tr}^2 A - 3\operatorname{ch} A)\sqrt{\operatorname{tr}^2 A - 3\operatorname{ch} A} - \operatorname{tr} A(2\operatorname{tr}^2 A - 9\operatorname{ch} A)}{27}$, *four roots;*

$\operatorname{ch} A > \operatorname{tr}^2 A/4$,

$\det A \geq 0$, *four roots;*

In all the cases stated above the real square roots S of A with $\det S \geq 0$ are given by

$$S = \frac{4}{p_A'(\tau)}\left(-2A^2 + (\tau^2 + \operatorname{tr} A)A + 2\sqrt{\det A}\,\tau I\right) \tag{18}$$

where τ is any simple real root of the polynomial

$$p_A(\lambda) = \lambda^4 - 2(\operatorname{tr} A)\lambda^2 - 8\sqrt{\det A}\,\lambda + \operatorname{tr}^2 A - 4\operatorname{ch} A, \tag{19}$$

b) If the minimal polynomial of A has degree 2 then all the eigenvalues of A are real so it suffices to assume that A is in Jordan canonical form. Two sub-cases arise:

b_1) A has only one real eigenvalue with algebraic multiplicity 3, in which case A admits real square roots if and only if the eigenvalue is non-negative.

Specifically, $A = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 1 \\ 0 & 0 & \alpha \end{bmatrix}$, $\alpha \geq 0$, *admits the infinite family of real square roots S given by, for arbitrary $p, q \in \mathbf{R}$,*

$$\begin{cases} \begin{bmatrix} 0 & 0 & 1/p \\ p & 0 & q \\ 0 & 0 & 0 \end{bmatrix}, \ p \neq 0, & \text{if } \alpha = 0, \\ \pm \begin{bmatrix} -\sqrt{\alpha} & 0 & q \\ p & \sqrt{\alpha} & (1-pq)/(2\sqrt{\alpha}) \\ 0 & 0 & \sqrt{\alpha} \end{bmatrix}, \pm \begin{bmatrix} \sqrt{\alpha} & 0 & 0 \\ 0 & \sqrt{\alpha} & 1/(2\sqrt{\alpha}) \\ 0 & 0 & \sqrt{\alpha} \end{bmatrix}, & \text{if } \alpha > 0. \end{cases} \tag{20}$$

b_2) A has two distinct real eigenvalues, one with algebraic multiplicity 1 and the other one with algebraic, and also geometric, multiplicity 2, in which case A admits real square roots if and only if the eigenvalue of multiplicity 1 is non-negative.

Specifically, $A = \operatorname{diag}(\alpha, \beta, \beta)$, $\alpha, \beta \in \mathbf{R}$, $\alpha \neq \beta$, $\alpha \geq 0$, *admits the infinite family of square roots S given by*

$$S = \begin{bmatrix} \pm\sqrt{\alpha} & 0 & 0 \\ 0 & p & q \\ 0 & (\beta - p^2)/q & -p \end{bmatrix}, \ p, q \in \mathbf{R}, q \neq 0, \tag{21}$$

to which we add the family $S = \begin{bmatrix} \pm\sqrt{\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & p & 0 \end{bmatrix}$, $p \in \mathbf{R}$, *if $\beta = 0$, and the family* $S = \pm \begin{bmatrix} \pm\sqrt{\alpha} & 0 & 0 \\ 0 & \sqrt{\beta} & 0 \\ 0 & p & -\sqrt{\beta} \end{bmatrix}$, *plus the matrices* $S = \pm \begin{bmatrix} \pm\sqrt{\alpha} & 0 & 0 \\ 0 & \sqrt{\beta} & 0 \\ 0 & 0 & \sqrt{\beta} \end{bmatrix}$, *if $\beta > 0$.*

c) If $A = aI$, $a \in \mathbf{R}$, then A admits (infinitely many) real square roots S if and only if $a \geq 0$, and

$$S = \begin{cases} uv^T, \quad u, v \in \mathbf{R}^3, u \cdot v = 0, & \text{if } a = 0, \\ \pm\sqrt{a}I \quad \text{or} \quad \pm \sqrt{a}\left(I - uv^T\right), u, v \in \mathbf{R}^3, u \cdot v = 2, & \text{if } a > 0. \end{cases} \tag{22}$$

Proof. *a*) Notice that when a real 3×3 matrix A whose minimal polynomial has degree 3 admits real square roots S (with $\det S \geq 0$) Equation (11) prevents $\operatorname{tr} S$ from being a multiple zero of $p_A(\lambda)$. This and Equation (12) guarantee that A possesses only finitely many square roots, in fact exactly twice the number of distinct zeros of $p_A(\lambda)$. The proof of *a*) is then a simple consequence of the two theorems presented earlier.

b) If a real 3×3 matrix A has minimal polynomial of degree 2 then all its eigenvalues are real. This is because A has always a real eigenvalue, which must be a zero of the minimal polynomial. Therefore, the minimal polynomial has only real zeros and so does the characteristic polynomial, which is a multiple of degree 3 of it. Consequently, the Jordan canonical form of A and the matrix which conjugates A to its Jordan form are real matrices.

By degree minimality, A can have one distinct eigenvalue, say α, in which case its Jordan canonical form is forced to be $\begin{bmatrix}\alpha & 0 & 0\\ 0 & \alpha & 1\\ 0 & 0 & \alpha\end{bmatrix}$, or two distinct eigenvalues, $\alpha \neq \beta$, leading to the Jordan canonical form $\operatorname{diag}(\alpha, \beta, \beta)$.

Without loss of generality we proceed as if A were already in Jordan canonical form. It is possible to settle the real square root query directly, without reference to associated quartic polynomials. However, the interested reader can compare things for consistency.

b_1) For $A = \begin{bmatrix}\alpha & 0 & 0\\ 0 & \alpha & 1\\ 0 & 0 & \alpha\end{bmatrix}$, $\alpha \geq 0$ is a necessary condition for the existence of real square roots. It is also sufficient. To see this, assign to a real square root S the block form

$$S = \begin{bmatrix}-\sigma & v^T\\ u & \Sigma\end{bmatrix}, \quad \sigma \in \mathbf{R},\ u, v \in \mathbf{R}^2,\ \Sigma \in \operatorname{Mat}(2, \mathbf{R}). \tag{23}$$

Then $S^2 = A$ is equivalent to

$$\begin{cases}\sigma^2 + v^T u = \alpha\\ \Sigma u - \sigma u = 0,\ v^t\Sigma - \sigma v^T = 0\\ \Sigma^2 + uv^T = \begin{bmatrix}\alpha & 1\\ 0 & \alpha\end{bmatrix}\end{cases} \tag{24}$$

It follows from the last equation in (24) that $\Sigma^2 u + u(v^T u) = \begin{bmatrix}\alpha & 1\\ 0 & \alpha\end{bmatrix} u$, which via the first two equations (24) is equivalent to $u = p\begin{bmatrix}1\\ 0\end{bmatrix}$, $p \in \mathbf{R}$. Similarly,

$v^T\Sigma^2 + (v^T u)v^T = v^T \begin{bmatrix} \alpha & 1 \\ 0 & \alpha \end{bmatrix}$ leads to $v = q \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $q \in \mathbf{R}$. Thus, $v^T u = 0$, so $\sigma^2 = \alpha$, and also the last equation (24) becomes $\Sigma^2 = \begin{bmatrix} \alpha & 1-pq \\ 0 & \alpha \end{bmatrix}$.

By [1], $\begin{bmatrix} \alpha & 1-pq \\ 0 & \alpha \end{bmatrix}$ admits real 2×2 square roots Σ if and only if $\alpha > 0$, or $\alpha = 0$ and $pq = 1$.

If $\alpha > 0$ there are two possible square roots, $\Sigma = \pm \begin{bmatrix} \sqrt{\alpha} & (1-pq)/(2\sqrt{\alpha}) \\ 0 & \sqrt{\alpha} \end{bmatrix}$ The diagonal entries of Σ must equal σ if $\begin{bmatrix} p \\ q \end{bmatrix} \neq 0$ and are independent of σ if $\begin{bmatrix} p \\ q \end{bmatrix} = 0$. The second part of (20) follows.

If $\alpha = 0$ and necessarily $pq = 1$ then $\sigma = 0$, $\Sigma^2 = 0$, $\Sigma \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0$, and $\Sigma^T \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0$. Therefore, $\Sigma = \begin{bmatrix} 0 & r \\ 0 & 0 \end{bmatrix} = 0$, $r \in \mathbf{R}$. This gives the first part of (20).

b_2) When $A = \mathrm{diag}(\alpha, \beta, \beta)$, $\alpha, \beta \in \mathbf{R}$, $\alpha \neq \beta$, the same approach as in b_1) based on the block representation (23) of a square root S of A leads to $u = v = 0$. Therefore, $S = \mathrm{diag}(-\sigma, \Sigma)$, with $\sigma^2 = \alpha$ and $\Sigma^2 = \beta I$.

Consequently, $\alpha \geq 0$ is a necessary condition for the existence of square roots. It is easy to see now (cf. also [1]) that any real 2×2 matrix Σ satisfying $\Sigma^2 = \beta I$ must belong to the infinite family

$$\Sigma = \begin{bmatrix} p & q \\ (\beta - p^2)/q & -p \end{bmatrix}, \ p, q \in \mathbf{R}, q \neq 0, \tag{25}$$

to which we add the family $\Sigma = \begin{bmatrix} 0 & 0 \\ p & 0 \end{bmatrix}$, $p \in \mathbf{R}$, if $\beta = 0$, and the family $\Sigma = \pm \begin{bmatrix} \sqrt{\beta} & 0 \\ p & -\sqrt{\beta} \end{bmatrix}$, plus the two matrices $\Sigma = \pm\mathrm{diag}(\sqrt{\beta}, \sqrt{\beta})$, if $\beta > 0$.

This proves b_2).

c) When $A = aI$, $a \in \mathbf{R}$, $a \geq 0$ is a necessary condition for the existence of real square roots S. We treat separately the cases $a = 0$ and $a > 0$.

If $a = 0$, then $S^2 = 0$ implies that the null space of S contains the range of S, and so $\mathrm{rank}(S) \leq \mathrm{nullity}(S)$. Since $\mathrm{nullity}(S) + \mathrm{rank}(S) = 3$, $\mathrm{rank}(S) \leq 1$. So either $S = 0$ or $\mathrm{rank}(S) = 1$. In the latter case there are non-zero vectors $u, v \in \mathbf{R}^3$ such that $S = uv^T$. Then clearly $S^2 = 0$ is equivalent to $u \cdot v = 0$, which proves the upper half of c).

If $a > 0$, by replacing a square root S of aI with $1/\sqrt{a}S$ we conclude that there is no loss of generality in assuming $a = 1$. When $S^2 = I$, either $S = \pm I$

or else one of $S \pm I$ has rank 1, and the discussion continues as in the case $a = 0$, except that now u and v must be chosen such that $u \cdot v = 2$. This completes the proof of the corollary.

□

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