What Is a Matrix Square Root?

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A square root of an $n \times n$ matrix A is any matrix X such that $X^2 = A$.

For a scalar a ($n = 1$), there are two square roots (which are equal if $a = 0$), and they are real if and only if a is real and nonnegative. For $n \geq 2$, depending on the matrix there can be no square roots, finitely many, or infinitely many. The matrix

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

is easily seen to have no square roots. The matrix

$$D = \operatorname{diag}(1, 2) = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

has four square roots, $\operatorname{diag}(\pm 1, \pm\sqrt{2})$. The identity matrix

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

has infinitely many square roots (namely the 2×2 involutory matrices), including $\operatorname{diag}(\pm 1, \pm 1)$, the lower triangular matrix

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

and any symmetric orthogonal matrix, such as

$$\begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix}, \quad \theta \in [0, 2\pi]$$

(which is a Householder matrix). Clearly, a square root of a diagonal matrix need not be diagonal.

The matrix square root of most practical interest is the one whose eigenvalues lie in the right half-plane, which is called the *principal square root*, written $A^{1/2}$. If A is nonsingular and has no eigenvalues on the negative real axis then A has a unique principal square root. For the diagonal matrix D above, $D^{1/2} = \operatorname{diag}(1, \sqrt{2})$.

A symmetric positive definite matrix has a unique symmetric positive definite square root. Indeed if A is symmetric positive definite then it has a spectral decomposition

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$A = QDQ^T$, where Q is orthogonal and D is diagonal with positive diagonal elements, and then $A^{1/2} = QD^{1/2}Q^T$ is also symmetric positive definite.

If A is nonsingular then it has at least 2^s square roots, where s is the number of distinct eigenvalues. The existence of a square root of a singular matrix depends on the Jordan structure of the zero eigenvalues.

In some contexts involving symmetric positive definite matrices A, such as Kalman filtering, a matrix Y such that $A = Y^TY$ is called a square root, but this is not the standard meaning.

When A has structure one can ask whether a square root having the same structure, or some other related structure, exists. Results are known for (for example)

- stochastic matrices,
- M-matrices,
- skew-Hamiltonian matrices,
- centrosymmetric matrices, and
- matrices from an automorphism group.

An important distinction is between square roots of A that can be expressed as a polynomial in A (primary square roots) and those that cannot. Square roots of the latter type arise when A has repeated eigenvalues and two copies of an eigenvalue are mapped to different square roots. In some contexts, a nonprimary square root may be the natural choice. For example, consider the matrix

$$G(\theta) = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}, \quad \theta \in [0, 2\pi],$$

which represents a rotation through an angle θ radians clockwise. The natural square root of $G(\theta)$ is $G(\theta/2)$. For $\theta = \pi$, this gives the square root

$$G(\pi/2) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

of

$$G(\pi) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The matrix square root arises in many applications, often in connection with other matrix problems such as the polar decomposition, matrix geometric means, Markov chains (roots of transition matrices), quadratic matrix equations, and generalized eigenvalue problems. Most often the matrix is symmetric positive definite, but square roots of nonsymmetric matrices are also needed. Among modern applications, the matrix square root can be found in recent papers on machine learning.

References

This is a minimal set of references, which contain further useful references within.

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