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THE SQUARE ROOT OF A MATRIX

The square root of a matrix

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Abstract

This note derives an explicit formula for the numerical calculation of the square root of a matrix, when this function exists. An example is given as an illustration of the formula. The condition for the existence of the square root is also given.

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1. Introduction.

The square root of a matrix is usually written implicitly, explicit formulae being available only in the symmetric case. Calculating it is often required in econometrics and statistics, even for asymmetric matrices; for example, in the analysis of a multivariate ARCH model

$$\mathrm{vech}(\boldsymbol{\Sigma}_t) = \boldsymbol{\delta} + \boldsymbol{\Gamma}\,\mathrm{vech}(\boldsymbol{y}_{t-1}\boldsymbol{y}'_{t-1}),$$

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where $\boldsymbol{\Sigma}_t$ denotes the conditional variance, $\mathrm{E}(\boldsymbol{y}_t \mid \boldsymbol{y}_{t-1}) = \mathbf{0}$, and the square $\boldsymbol{\Gamma}$ need not be symmetric. Therefore, it is of interest to have a general explicit formula for the square-root function. This note does so.

The plan of the note is as follows. I start by considering the square root as the single-valued function defined on $\mathbb{R}_{0,+} \to \mathbb{R}_{0,+}$, the nonnegative real numbers. This is the most common usage of the function (the "principal value" in the language of complex analysis) and it is straightforward to extend it to positive semidefinite matrices. Then, the corresponding extension to general square matrices is given in (1)–(4), the latter being obtained explicitly for the first time. It is followed by conditions for the existence of the square-root function in the case of matrices. The notation conventions proposed in Abadir and Magnus (2002) are used.

2. Square root.

Start with the diagonal matrix

$$\boldsymbol{\Lambda} = \begin{pmatrix} 4 & 0 \\ 0 & 9 \end{pmatrix} \equiv \mathrm{diag}(4, 9).$$

There are four matrices which satisfy the equation $\boldsymbol{D}^2 = \boldsymbol{\Lambda}$, namely

$$\boldsymbol{D}_1 := \mathrm{diag}(-2, -3), \quad \boldsymbol{D}_2 := \mathrm{diag}(-2, 3),$$
$$\boldsymbol{D}_3 := \mathrm{diag}(2, -3), \quad \boldsymbol{D}_4 := \mathrm{diag}(2, 3),$$

but only $\boldsymbol{D}_4$ is the square root of $\boldsymbol{\Lambda}$ that is compatible with the one-dimensional definition given earlier. Hence, the matrix function $\boldsymbol{\Lambda}^{1/2}$ is uniquely defined for any diagonal matrix with nonnegative elements on the diagonal.

Next consider a symmetric (hence real) matrix $\boldsymbol{A}$. This matrix can be diagonalized so that $\boldsymbol{A} = \boldsymbol{S\Lambda S}'$, where $\boldsymbol{S}$ is orthogonal and $\boldsymbol{\Lambda}$ is diagonal. In accordance with the usual definition of matrix functions for symmetric matrices, define $\boldsymbol{A}^{1/2} := \boldsymbol{S\Lambda}^{1/2}\boldsymbol{S}'$. Here, $\boldsymbol{\Lambda}^{1/2}$ is defined exactly as before because $\boldsymbol{\Lambda}$ has nonnegative diagonal elements. Hence, for any positive semidefinite matrix $\boldsymbol{A}$, there exists a unique positive semidefinite matrix $\boldsymbol{B}$ such that $\boldsymbol{B}^2 = \boldsymbol{A}$; this unique matrix is called the square root of $\boldsymbol{A}$. If $\boldsymbol{A}$ is positive definite (hence nonsingular), then the notation $\boldsymbol{A}^{-1/2}$ denotes the inverse of $\boldsymbol{A}^{1/2}$ or the square root of $\boldsymbol{A}^{-1}$ — they are the same.

Can one also define a unique square root for nonsymmetric real matrices? Yes, this is possible when the eigenvalues are positive. Consider a real $n \times n$ matrix $\boldsymbol{A}$ with positive eigenvalues $\lambda_1, \dots, \lambda_n$, not necessarily distinct. Denote by $\boldsymbol{J}_m(\lambda)$ a Jordan block, that is, a $m \times m$ matrix of the form

$$\boldsymbol{J}_m(\lambda) := \begin{pmatrix} \lambda & 1 & 0 & \dots & 0 \\ 0 & \lambda & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ 0 & 0 & 0 & \dots & \lambda \end{pmatrix}.$$

(For $m = 1$, let $J_1(\lambda) := \lambda$.) Jordan's decomposition theorem then guarantees the existence of a nonsingular $n \times n$ matrix $\boldsymbol{T}$ such that $\boldsymbol{T}^{-1}\boldsymbol{AT} = \boldsymbol{J}$, where

$$\boldsymbol{J} := \begin{pmatrix} \boldsymbol{J}_{n_1}(\lambda_1) & 0 & \dots & 0 \\ 0 & \boldsymbol{J}_{n_2}(\lambda_2) & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \boldsymbol{J}_{n_k}(\lambda_k) \end{pmatrix} \tag{1}$$

with $n_1 + n_2 + \cdots + n_k = n$; see Section 7.6 of Abadir and Magnus (2005) for the explicit method of constructing the matrices in this decomposition.

The square root of $\boldsymbol{A}$ can now be defined through its Jordan representation $\boldsymbol{A} = \boldsymbol{TJT}^{-1}$ as

$$\boldsymbol{A}^{1/2} := \boldsymbol{TJ}^{1/2}\boldsymbol{T}^{-1}, \tag{2}$$

where $\boldsymbol{J}^{1/2} := \operatorname{diag}\left(\boldsymbol{J}_{n_1}^{1/2}(\lambda_1), \ldots, \boldsymbol{J}_{n_k}^{1/2}(\lambda_k)\right)$ and

$$\boldsymbol{J}_{n_i}^{1/2}(\lambda_i) := \begin{pmatrix} \lambda_i^{1/2} & g_1(\lambda_i) & \ldots & g_{n_i-1}(\lambda_i) \\ 0 & \lambda_i^{1/2} & \ldots & g_{n_i-2}(\lambda_i) \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \ldots & \lambda_i^{1/2} \end{pmatrix} \tag{3}$$

for $i = 1, \ldots, k$. The functions g_j are scaled derivatives of $f(\lambda) := \lambda^{1/2}$ (see p.260 of Abadir and Magnus, 2005), and specialize here to

$$g_j(\lambda) := \frac{f^{(j)}(\lambda)}{j!} = \binom{1/2}{j}\lambda^{1/2-j}, \tag{4}$$

where the binomial coefficients are given by

$$\binom{1/2}{j} = \frac{\prod_{i=0}^{j-1}\left(\frac{1}{2} - i\right)}{j!}.$$

For example,

$$\begin{pmatrix} 3 & 1 & 0 \\ 0 & 3 & 1 \\ 0 & 0 & 3 \end{pmatrix}^{1/2} = \sqrt{3}\begin{pmatrix} 1 & 1/6 & -1/72 \\ 0 & 1 & 1/6 \\ 0 & 0 & 1 \end{pmatrix}.$$

The result given in Abadir and Magnus (2005) applies here because $f(\lambda) := \lambda^{1/2}$ has a power series expansion that is summable (but not necessarily convergent) for $\lambda \neq 0$.

This brings us to two further questions: what if $\lambda = 0$ and what if the definition is extended to $\lambda \notin \mathbb{R}_{0,+}$ (such as real negative λ and/or complex λ)?

First, for $\lambda = 0$ the matrix $\boldsymbol{A}^{1/2}$ may not exist. The simplest example is the matrix $\boldsymbol{J}_2(0)$, which has no square root because the matrix equation

$$\boldsymbol{X}^2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

has no solution. More generally, the matrix $\boldsymbol{J}_m(0)$ has no square root when $m > 1$, because the matrix is nilpotent and its index is equal to its dimension. (If a square matrix $\boldsymbol{J}$ of any dimension satisfies $\boldsymbol{J}^{m-1} \neq \mathbf{O}$ and $\boldsymbol{J}^m = \mathbf{O}$, then $\boldsymbol{J}$ is nilpotent of index m.) Clearly, the square root of $J_1(0) = 0$ exists. But the square root exists also if one can pair a block like $\boldsymbol{J}_m(0)$ with another block $\boldsymbol{J}_m(0)$ or $\boldsymbol{J}_{m\pm 1}(0)$ in the decomposition of $\boldsymbol{A}$. The effect of the latter pairing can be illustrated with

$$\operatorname{diag}(\boldsymbol{J}_2(0), J_1(0)) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

This matrix can be transformed by a permutation matrix $\boldsymbol{P}$ and its transpose (inverse) to $\boldsymbol{P} \operatorname{diag}(\boldsymbol{J}_2(0), J_1(0))\boldsymbol{P}'$, thereby preserving the Jordan structure $\boldsymbol{A} = \boldsymbol{T}\boldsymbol{J}\boldsymbol{T}^{-1}$. Choosing

$$\boldsymbol{P} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

the result of the transformation is a nilpotent matrix of index 2 whose square root exists (since the index is less than the dimension) and is nilpotent of index 3. More specifically,

$$\left(\boldsymbol{P}\begin{pmatrix}\boldsymbol{J}_2(0) & 0\\ 0 & J_1(0)\end{pmatrix}\boldsymbol{P}'\right)^{1/2} = \begin{pmatrix}0 & 0 & 1\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}^{1/2} = \begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 1\\ 0 & 0 & 0\end{pmatrix} = \boldsymbol{J}_3(0),$$

and hence

$$\begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}^{1/2} = \begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}\begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix} = \begin{pmatrix}0 & 0 & 1\\ 0 & 0 & 0\\ 0 & 1 & 0\end{pmatrix}.$$

Similarly, if one can pair two blocks $\boldsymbol{J}_m(0)$ in the decomposition of $\boldsymbol{A}$, then the square root exists too. If all Jordan blocks having $\lambda = 0$ can be paired in one of these two ways, with a leftover block (if any) of the form $J_1(0) = 0$, then the square root of the matrix will exist uniquely for all $\lambda \in \mathbb{R}_{0,+}$.

Second, the result of (3)–(4) is applicable to all $\lambda \neq 0$, by analytic continuation of the binomial expansion for all $\lambda \in \mathbb{C}\backslash\{0\}$. However, in this case, one has to be careful to choose the principal value of the square roots in (3)–(4). For example, the principal values of $\sqrt{4}$ and $\sqrt{-4}$ are 2 and 2i, respectively, and not -2 and -2i. This extension is applicable to complex matrices, as well as real matrices with complex eigenvalues.

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References

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