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Computing the Square Root of an Tridiagonal Toeplitz Matrix

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Abstract

In this article a numerical algorithm is introduced for computing the square root of a square matrix. The algorithm depends mainly on Newton's iteration method together witheig envalues and eigenfunctions of the square matrix. The algorithm will be used for computing the square root $B^{\frac{1}{2}}$ of an $n \times n$ square matrix *B*, where *B* is an Tridiagonal Toeplitz or Semidefinite square matrix arising normally from the numerical algorithms for solving ordinary, partial differential equations and statistics. The QR algorithm will be used to compute the eigenvalues of the matrix. Jameson's method will be used in solving equations of the form $AX + BX = C$ results in Newton's algorithm. The algorithm is implemented and simulated in the mathematical code MATLAB with double precision calculations and implicit formulas with a close initial matrix. Numerical results show that the computed square root of Tridiagonal Toeplitz or Semidefinite matrix is a persymmetric matrix, where its symmetric across lower-left to upper-right diagonal, the obtained results agree well and consistent with results from explicit analytical calculations.

AMS Subject Classification: 15A09

Keywords: Square root, Newton's method, Jameson's method, QR algorithm, Tridiagonal Toeplitz matrix, Semidefinite matrix, Eigenvalues, Eigenvectors.

1. INTRODUCTION

There are many numerical algorithms for computing the roots of non-linear functions, bisection, false position, secant, fixed point , Newton's … etc. [5, 6, 7] The most used method in applied sciences and engineering is Newton's algorithm, it's widely used for its simplicity and high rate of convergence. The general formula of Newton's method is,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \qquad n= 0, 1,2,3,\ldots \qquad (1)$$

Where, x_0 is a given initial value. For the quadratic equation $x^2 - b = 0, \quad b \in \mathbb{C}$ the above formula turns into

$$x_{n+1} = \frac{x_n + \frac{b}{x_n}}{2}, \qquad n= 0,1,2,3\ldots. \qquad (2)$$

$x_\circ \approx \sqrt{b}$

The above formula is quadratically convergent, and is usually used to approximate the square roots of any real number *b.*

Similar formula can be derived as well to approximate the cubic roots. The general algorithm for the P^{th} root is,

$$x_{n+1} = \frac{(p-1)x_n + b x_n^{1-p}}{p}, \qquad n=0,1,2,\ldots \qquad (3)$$

The square root of a matrix extends the notion of square root from numbers to matrices. A matrix *X* is said to be a square root of *B* if the matrix product *XX* is equal to *B*.

The iterative method in (3) can be extended to matrices. Consider the $n \times n$ matrix $B \in \mathbb{C}^{n\times n}$, we can solve the matrix equation

$X^P - B = 0,$

using the matrix iteration formula with the identity matrix as the initial matrix value $X_\circ = \mathrm{I}$,

$$X_{n+1} = \frac{(p-1)X_n + B X_n^{1-p}}{p}, \qquad n= 0, 1, 2, \ldots \qquad (4)$$

The general Newton formula for the matrix root is [7]:

$$X_{n+1} = X_n - F_{X_n}'^{-1}\big(F(X_n)\big),$$

Where X_n are well defined, and F_{X_n}' is the Frechet derivative at X_n [7].

If $F'(X)$ is nonsingular and $\|X - X_\circ\|$ is sufficiently small, then Newton iteration method will converge quadratically to a square root *X* of the original matrix *B*.[5, 9]

For *P=2*, the formula in (4) referred as the Babylonian method, or as Heron's method [4],

$$X_{n+1} = \frac{X_n + B X_n^{-1}}{2}, \qquad n= 0,1, 2,\ldots \qquad (5)$$

The method is based on a historical method of calculating square roots, [4] it was defined for the first time in the first century by Hero of Alexandria. [4] Some authors use the name square root or the notation $B^{1/2}$ only for the specific case when *B* is positive semidefinite, to denote the unique matrix X that is positive semidefinite and such that $XX = X^{T}X = B$ (for real-valued matrices, where X^{T} is the transpose of X).

Denman–Beavers square root iteration is another well known iterative numerical methods of approximating the square root of a real or complex $n \times n$ matrix [3]. One of the disadvantages of both iterative methods is that, convergence is not guaranteed, but if the process converges, the computed matrix converges quadratically to a square root $B^{1/2}$. Also such methods may fail to find a root even if such root exists, and will only find a single root.

If $n \times n$ matrix is diagonalizable, it has been shown to always have P^{th} roots [7], for any integer P. For non-diagonalizable matrices [14, 15, 16], as specifically in the case of nilpotent matrices, the roots may exist only for specific value of P , and there may be no P^{th} roots. If B is a positive semidefinite matrix (real or complex) [1, 14]. Then there is exactly one positive square root matrix.

In this paper Newton's algorithm in combination with Jameson's algorithm [5], will be used to approximate the square root of tridiagonal Toeplitz matrix. Jameson's method will be used in solving equation of the form $AX + BX=C$ results in Newton's algorithm [7]. It will be shown that the square root of tridiagonal Toeplitz matrix has the form of a persymmetric matrix.

Definition 1 A square real matrix B is positive semidefinite if and only if $B = X^{T}X$ for some matrix X. All eigenvalues of the positive semidefinite matrix are non-negative.

Definition 2 The Nilpotent matrix is a matrix that when taken to some power n becomes zero matrix. For $n \times n$ matrix B,

$$B^{n} = [\mathbf{0}]$$

The minimum value of n for which A^{n} is the zero matrix is called the index of the Nilpotent matrix.

2. ROOTS OF THE THE TRIDIAGONAL TOEPLITZ MATRIX

Tridiagonal Toeplitz matrices and low-rank perturbations of such matrices arise in numerous applications, including the solution of ordinary and partial differential equations [9, 10, 13], time series analysis [13]. It is therefore important to understand properties of tridiagonal Toeplitz matrices relevant for computation.

The general form of Tridiagonal Toeplitz 6×6 matrix B is illustrated below:

$$\boldsymbol{B}= \begin{bmatrix} c & a & 0 & 0 & 0 & 0 \\ b & c & a & 0 & 0 & 0 \\ 0 & b & c & a & 0 & 0 \\ 0 & 0 & b & c & a & 0 \\ 0 & 0 & 0 & b & c & a \\ 0 & 0 & 0 & 0 & b & c \end{bmatrix} \quad a \neq 0, b \neq 0$$

Definition 3 an $n \times n$ matrix $B \in R^{n\times n}$ is said to be a persymmetric matrix if its symmetric across lower-left to upper-right diagonal such that

$b_{ij} = b_{n-j+1,n-i+1}$, *i, j= 1,2,…,n*

For example, 6 × 6 persymmetric matrices are of the form

$$\boldsymbol{B}=\begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{16} \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} & b_{15} \\ b_{31} & b_{32} & b_{33} & b_{23} & b_{24} & b_{14} \\ b_{41} & b_{42} & b_{23} & b_{33} & b_{23} & b_{13} \\ b_{51} & b_{52} & b_{42} & b_{32} & b_{22} & b_{12} \\ b_{61} & b_{51} & b_{41} & b_{31} & b_{21} & b_{11} \end{bmatrix}$$

3. NUMERICAL METHOD

In the last few years there has been a significant increasing interest in developing the theory and numerical methods for the matrix square roots of Tridiagonal Toeplitz square matrices. The analytical formula of the matrix square root of Tridiagonal Toeplitz square matrices can be found in [9] . To apply Newton iteration method to find the square root of a matrix, we consider the square matrices *X*, $B \in R^{n\times n}$,

and *F* is defined as:

$$F(X) = X^2 - B$$

$$F(X+G) = X^2 - B + (XG + GX) + G^2 \qquad (6)$$

With the Taylor's series expansion of $F(X)$,

$$F(X+G) = F(X) + F'(X)G + \frac{F''(X)}{2!}G^2 + \cdots, \qquad (7)$$

$$F'(X)G = XG + GX, \qquad (8)$$

$$F''(X) = 2, \qquad (9)$$

$$X_{n+1} = X_n + G_n \quad n = 0,\ 1,\ 2,\ \ldots \qquad (10)$$

G_n is the solution of the equation

$$X_nG_n + G_nX_n = B - X_n^2, \qquad (11)$$

Equation (11) can be solved using Jameson's method [8], where *X* can be reduced to diagonal form as:

$$U^{-1}XU = \begin{pmatrix} \mu_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mu_n \end{pmatrix}$$

Where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of *X* , and *U* is $n \times n$ matrix where its columns are the corresponding eigenfunctions, then *G* is

$$G = U\,G^*\,U^{-1} \tag{12}$$

$$G^*_{ij} = \frac{C^*_{ij}}{\mu_i + \mu_j}$$

$$C^* = U^{-1}(B - X^2)U$$

Numerical algorithm for roots of the the Tridiagonal Toeplitz matrix

1. Given $X_\circ$ as initial value for the square root of the matrix *B*,
2. Use the QR algorithm to compute the eigenvalues of the matrix X, $\mu_1, \mu_2, \dots, \mu_n$
   - Compute $X_k = Q_k R_k$, Q_k is orthogonal matrix ($Q_T = Q^{-1}$)
     R_k is an upper triangular matrix,
   - $X_{k+1} = R_k\,Q_k = Q_k^{-1} Q_k R_k\,Q_k = Q_k^{-1} X_k Q_k = Q_k^{T} X_k Q_k$

   The matrices X_k converge to a triangular matrix, the Schur form of *X*. The eigenvalues of a triangular matrix are listed on the diagonal,
3. Compute the corresponding eigenfunctions matrix U,
4. Use Gaussian elimination algorithm to compute U^{-1}
5. Compute C^*_{ij} from the relation $C^* = U^{-1}(B - X^2)U$
6. Compute $G^*_{ij} = \frac{C^*_{ij}}{\mu_i + \mu_j}$
7. $X_{n+1} = X_n + G_n$ *n= 0, 1, 2, ...*

4. NUMERICAL COMPUTATIONS

The above numerical steps are implemented and simulated in the mathematical code MATLAB [11], a double precision calculations are used to reduce round-off error and to avoid unstability of the method, and the initial matrix is chosen such that $\|X - X_\circ\|$ is sufficiently small, the method is simulated for the following tridiagonal Toeplitz 6×6 matrix *B* and semidefinite positive matrix. The eigenvalues of real and complex tridiagonal Toeplitz matrices can be very sensitive to perturbations of the matrix [10]. So we used explicit formulas for the eigenvalues and eigenvectors of tridiagonal Toeplitz matrices.

Example 1:

Consider the following tridiagonal Toeplitz 6×6 matrix B

$$B = \begin{bmatrix} 4 & 2 & 0 & 0 & 0 & 0 \\ 1 & 4 & 2 & 0 & 0 & 0 \\ 0 & 1 & 4 & 2 & 0 & 0 \\ 0 & 0 & 1 & 4 & 2 & 0 \\ 0 & 0 & 0 & 1 & 4 & 2 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

The computed square root matrix of B is the persymmetric square matrix:

$$\text{Square root of } B = \begin{bmatrix} 1.9658 & 0.5184 & -0.0718 & 0.0203 & -0.0072 & 0.0026 \\ 0.2592 & 1.9299 & 0.5285 & -0.0754 & 0.0216 & -0.0072 \\ -0.0179 & 0.2643 & 1.9281 & 0.5292 & -0.0754 & 0.0203 \\ 0.0025 & -0.0188 & 0.2646 & 1.9281 & 0.5285 & -0.0718 \\ -0.0004 & 0.0027 & -0.0188 & 0.2643 & 1.9299 & 0.5184 \\ 0.0001 & -0.0004 & 0.0025 & -0.0179 & 0.2592 & 1.9658 \end{bmatrix}$$

Example 2:

Consider the following semidefinite 3×3 matrix H

$$H = \begin{bmatrix} 2 & -1 & 1 \\ -1 & 2 & -1 \\ 1 & -1 & 2 \end{bmatrix}$$

$$\text{Square root of } H = \begin{bmatrix} 1.3333 & -0.3333 & 0.3333 \\ -0.3333 & 1.3333 & -0.3333 \\ 0.3333 & -0.3333 & 1.3333 \end{bmatrix}$$

5. CONCLUSIONS

In this article it has been indicated that the diagonalizable matrices has P^{th} roots, for any integer p. for non-diagonalizable matrices, as in the case of nilpotent matrices, there may be no P^{th} root, or roots may exist only for specific values of p. There are many iterative methods for finding the roots of matrices, the most famous ones are, Denman–Beavers and Newton's square root iteration methods [3]. Although these methods may fail to find a root even if it exists, but in case of convergence, both methods converges quadratically to the root as in the case of roots of non-linear functions. It has been shown that, using double precision calculations, explicit formulas, close initial matrix to the root, and non-zero first derivative, Newton's method converge to the square root of the square matrix, if it's used with Jameson's method for solving equation of the form $AX + BX=C$.[2, 8] As an example it's shown that the tridiagonal Toeplitz has the form of persymmetric square matrix. Same procedure can be used to study properties of other diagonalizable matrices. The obtained computational results agree well with the theoretical results obtained by Krim in [9].

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