UDC 519.614

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NEWTON'S METHOD FOR THE EIGENVALUE PROBLEM OF A SYMMETRIC MATRIX

Newton's method for calculating the eigenvalue and the corresponding eigenvector of a symmetric real matrix is considered. The nonlinear system of equations solved by Newton's method consists of an equation that determines the eigenvalue and eigenvector of the matrix and the normalization condition for the eigenvector. The method allows someone to simultaneously calculate the eigenvalue and the corresponding eigenvector. Initial approximations for the eigenvalue and the corresponding eigenvector can be found by the power method or by the reverse iteration with shift. A simple proof of the convergence of Newton's method in a neighborhood of a simple eigenvalue is proposed. It is shown that the method has a quadratic convergence rate. In terms of computational costs per iteration, Newton's method is comparable to the reverse iteration method with the Rayleigh ratio. Unlike reverse iteration, Newton's method allows to compute the eigenpair with better accuracy.

MSC: 65F15.
Key words: Newton's method, eigenvalue, symmetric matrix, reverse iteration.
DOI: 10.18524/2519-206X.2020.2(36).233787.

1. Introduction

If a sufficiently good approximation to the solution of the equation $F(x) = 0$ is known, then the Newton method is an effective method for increasing the accuracy of approximation. Many statements about the convergence of Newton's method come from the well-known results of L.V. Kantorovich, who transferred Newton's method to nonlinear operator equations in Banach spaces[1].

The application of Newton's method to spectral problems of matrices has a long history. Without pretending to be complete, we can note some stages. J. H. Wilkinson [2] investigated the application of Newton's method to find the roots of the characteristic equation $det(A - \lambda I) = 0$. In the monograph by D.K. Faddeev. and V.N. Faddeeva [3] Newton's method is applicable to refine an individual eigenvalue and its own eigenvector, the first component of which is not vanishingly small in comparison with the others, so that without loss of generality it can be considered equal to unity. A nonlinear equation

Received 10.11.2020

is obtained for the eigenvalue. Newton's method is applied to this equation. In V. N. Kublanovskaya's article [4], an algorithm for finding the complex conjugate eigenvalues and eigenvectors of a real matrix in real arithmetic is constructed. To calculate the real and imaginary parts of the eigenvalue the roots of nonlinear equations are found by Newton's method. In all of the above cases, Newton's method was applied to scalar nonlinear equations to refine the required eigenvalue. L. Kollatz [5] described a different approach. The eigenvalue problem $Ax = \lambda Bx$ (A, B — given matrices of dimension $n \times n$) is reduced to finding the roots of a nonlinear system from the $n+1$ equation:

$$\begin{cases} Ax - \lambda Bx = 0, \\ x_n - 1 = 0. \end{cases} \tag{1}$$

To prove the convergence of Newton's method for system (1), it is proposed to use the theorem on the convergence of Newton's method for a nonlinear operator equation in a Banach space. However, in practice, it is difficult to prove the fulfillment of the conditions of this theorem. In the same place the proof of the convergence of Newton's method is given only for a numerical example with matrices of size 3×3. Moreover, the proof uses the estimates obtained on the basis of the values found in the process of calculations. The authors have not found any other proofs of the convergence of Newton's method for systems of the form (1). We have proposed a simple proof of the convergence of Newton's method for a system of the form (1), which is based on the known theorem on the convergence of Newton's method for a system of nonlinear equations [6].

2. Newton's method for the eigenvalue problem

The Newton method is introduced for the equation

$$F(x) = 0, \tag{2}$$

where $F : R^n \to R^n$ is a smooth mapping. Let $x^k \in R^n$ be the current approximation to the desired solution $\overline{x}$ of equation (2). Then the approximation x^{k+1} is found from the linear approximation of equation (2) near x^k,

$$F(x^k) + F'(x^k)(x - x^k) = 0,$$

and Newton's method is written as

$$x^{k+1} = x^k - (F'(x^k))^{-1} F(x^k), \quad k = 0, 1, \ldots. \tag{3}$$

In [6] the following theorem is proved.

Theorem 1. *Let the map $F : R^n \to R^n$ be differentiable in some neighborhood of the point $\overline{x} \in R^n$, and its derivative is continuous at this point. Let $\overline{x}$ be a solution to equation (2), and $\det F'(\overline{x}) \neq 0$. Then for any initial approximation $x^0 \in R^n$ sufficiently close to $\overline{x}$, Newton's method (3) defines a sequence converging to $\overline{x}$. The rate of convergence is superlinear, and if the derivative F is continuous in the Lipschitz sense in a neighborhood of the point $\overline{x}$, then it is quadratic.*

The eigenvalues and the corresponding eigenvectors of the symmetric matrix $A \in R^{n\times n}$ are the roots of the nonlinear system:

$$\begin{cases} Ax - \lambda x = 0, \\ \frac{1}{2}(1 - x^T x) = 0. \end{cases} \tag{4}$$

The last equation of the system is the normalization condition of the eigenvector. We write system (4) in the form (2), setting

$$F\left(\begin{bmatrix} x \\ \lambda \end{bmatrix}\right) = \begin{bmatrix} Ax - \lambda x \\ \frac{1}{2}(1 - x^T x) \end{bmatrix}. \tag{5}$$

The derivative of the mapping F is easy to calculate:

$$F'\left(\begin{bmatrix} x \\ \lambda \end{bmatrix}\right) = \begin{bmatrix} A - \lambda I & -x \\ -x^T & 0 \end{bmatrix}. \tag{6}$$

Let's define the following iterative process:

$$\begin{bmatrix} x^{k+1} \\ \lambda^{k+1} \end{bmatrix} = \begin{bmatrix} x^k \\ \lambda^k \end{bmatrix} - \left(F'\left(\begin{bmatrix} x^k \\ \lambda^k \end{bmatrix}\right)\right)^{-1} F\left(\begin{bmatrix} x^k \\ \lambda^k \end{bmatrix}\right), \quad k = 0, 1, \ldots. \tag{7}$$

Theorem 2. *Let $\overline{\lambda}$ be a simple eigenvalue, $\overline{x}$ be the corresponding eigenvector of a real symmetric matrix A. Then for any initial approximations $[x^0, \lambda^0]^T$ sufficiently close to $[\overline{x}, \overline{\lambda}]^T$, Newton's method (7) defines a sequence converging to $[\overline{x}, \overline{\lambda}]^T$ with quadratic speed.*

Proof. Let us show that for the mapping F of the iterative process (7) all conditions of Theorem 2 are satisfied. Indeed, according to (5) and (6), the mapping F is continuously differentiable, and its derivative is continuous in the Lipschitz sense in the neighborhood of $[\overline{x}, \overline{\lambda}]^T$. Let us prove that

$$\det F'\left(\begin{bmatrix} \overline{x} \\ \overline{\lambda} \end{bmatrix}\right) \neq 0.$$

It suffices to show that the system

$$\begin{bmatrix} A - \overline{\lambda} I & -\overline{x} \\ -\overline{x}^T & 0 \end{bmatrix} \begin{bmatrix} x \\ \lambda \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{8}$$

has only a trivial solution. Multiplying the first equation of system (8) on the left by x^T and taking into account the last equation, we obtain

$$x^T A x - \overline{\lambda} x^T x = 0.$$

If we assume that $x \neq 0$, then

$$\overline{\lambda} = \frac{x^T A x}{x^T x}$$

and $x = \alpha \overline{x}$ ($\alpha \neq 0$), because $\overline{\lambda}$ is a simple eigenvalue. But then from the last equation of system (8) $\alpha \overline{x}^T \overline{x} = 0$. It is impossible. Hence, $x = 0$. Taking this into account, the first equation of system (8) takes the form

$$-\lambda \overline{x} = 0.$$

Hence, $\lambda = 0$. □

Let λ^0, x^0 be some approximations to the required eigenpair $\overline{\lambda}$, $\overline{x}$ of a symmetric matrix A. Then, the k-th step of Newton's method (7) is conveniently written as follows:

1. find the solution $[y^k, \mu^k]^T$ of the system

$$\begin{bmatrix} A - \lambda^k I & -x^k \\ -(x^k)^T & 0 \end{bmatrix} \begin{bmatrix} y^k \\ \mu^k \end{bmatrix} = \begin{bmatrix} A x^k - \lambda^k x^k \\ \frac{1}{2}(1 - (x^k)^T x^k) \end{bmatrix}; \tag{9}$$

2. define

$$\begin{cases} x^{k+1} = x^k - y^k, \\ \lambda^{k+1} = \lambda^k - \mu^k. \end{cases}$$

Let us note some features of Newton's method (7). The right-hand side of Eq. (9) contains the residual $r^k = (A - \lambda^k)x^k$, which is the best computational measure of the accuracy of (λ^k, x^k) as an eigenpair of the matrix A [7]. Therefore, it is convenient to define the condition for the completion of the iterative process as follows:

$$||r^k|| \leq \varepsilon, \tag{10}$$

where ε is the required computational accuracy.

In terms of computational costs, Newton's method (7) is comparable to the reverse iteration with the Rayleigh ratio, the k-th step of which has the form [7]

$$\begin{aligned}
&1. \quad \rho^k = (x^k)^T A x^k,\\
&2. \quad (A - \rho^k)y^{k+1} = x^k,\\
&3. \quad x^{k+1} = y^{k+1}/||y^{k+1}||_2.
\end{aligned}$$

Indeed, at each iteration, the main computational costs of the methods are associated with solving the system, the matrix of which changes with the use of the shift λ^k or ρ^k. Newton's method may be preferable to reverse iteration with the Rayleigh ratio in the following case. If the eigenvalue is computed by reverse iteration with high precision, then the matrix $A - \rho^k I$ becomes degenerate in machine arithmetic and the calculations should be interrupted. It may happen that the corresponding eigenvector has not yet been calculated with a given precision. As proved above, the matrix of system (9) is nondegenerate, even if λ^k coincides with the desired eigenvalue. Therefore, calculations by Newton's method can be continued to achieve the required accuracy of the eigenvector even if the eigenvalue has already been calculated exactly.

3. Numerical experiments

The finite-difference approximation of the spectral problem for the Laplace operator in the unit rectangle with homogeneous Dirichlet conditions is an eigenvalue problem for the symmetric matrix A. All eigenvalues of the matrix A are different. The minimum eigenvalue and its corresponding eigenvector are defined as follows [8]:

$$\lambda_h = \frac{8}{h^2}\sin^2\frac{\pi h}{2},$$

$$\varphi_h(x_i, y_i) = 2\sin(\pi x_i)\sin(\pi y_i), \quad x_i = ih,\ y_j = jh,\ i, j = 1, \ldots, N-1.$$

Here the integer N defines the parameter $h = 1/N$ of the uniform mesh on the unit rectangle.

Calculations have been performed by the MATLAB package. The minimum eigenvalue and the corresponding eigenvector of the matrix A of size $10^5 \times 10^5$ ($N = 101$) have been calculated by the Newton method and inverse iteration with the Rayleigh ratio. To determine the initial approximations λ^0 and x^0, one step of reverse iteration had been performed for the initial vector $y^0 = [1, \dots, 1]^T$. The calculation results are presented in tables 1 and 2. Let's note the following. In three steps of reverse iteration with the Rayleigh relation, the matrix $A - \rho^h I$ becomes degenerate in machine arithmetic and the calculations are terminated. In Newton's method, the condition number of the matrix of system (9) does not increase when approaching the eigenvalue and calculations can be continued to achieve better accuracy.

Table 13: Reverse iteration with the Rayleigh ratio.

k	$\|\|r^k\|\|_2$	$\lambda_h - \rho^k$	$\|\|\varphi_h - x^k\|\|_2$	$cond(A - \rho^k I)$
1	12.2	-0.901	2.00	9.04e+04
2	0.0895	-9.64e-05	1.33e-09	8.46e+08
3	1.06e-07	-1.42e-14	*	6.08e+16

Table 14: Newton's method.

k	$\|\|r^k\|\|_2$	$\lambda_h - \lambda^k$	$\|\|\varphi_h - x^k\|\|_2$	$cond\left(\begin{bmatrix} A - \lambda^k I & -x^k \\ -(x^k)^T & 0 \end{bmatrix}\right)$
1	14.2	0.0874	0.0125	6.83e+05
2	0.900	5.04e-04	7.801e-05	8.47e+04
3	0.00108	3.88e-08	3.05e-09	8.16e+04
4	3.93e-08	-3.55e-14	1.84e-15	8.16e+04
5	4.25e-12	-7.11e-15	1.77e-15	8.16e+04

4. Conclusion

Newton's method for calculating the eigenvalue and the corresponding eigenvector of a symmetric real matrix is presented in this study. The proof of the quadratic rate convergence of Newton's method in a neighborhood of a simple eigenvalue is given. In terms of computational costs per iteration, Newton's method is comparable to the reverse iteration method with the Rayleigh ratio. The most attractive feature of this method is that it allows to compute the eigenpair with good accuracy. Proving of the applicability of the method for multiple eigenvalues and for asymmetric matrices is the prospects for further research in this direction.

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Метод Ньютона для задачі на власні значення симетричної матриці

Резюме

Розглянуто метод Ньютона обчислення власного значення та відповідного власного вектора дійсної симетричної матриці. Нелінійна система рівнянь, яка розв'язується методом Ньютона, складається з рівняння, що визначає власне значення і власний вектор матриці, та умови нормування власного вектора. Метод дозволяє одночасно обчислювати власне значення і відповідний власний вектор. Початкові наближення для власного значення і відповідного власного вектора можна знайти степеневим методом або методом зворотної ітерації зі зсувом. Запропоновано простий доказ збіжності методу Ньютона в околиці простого власного значення. Показано, що метод має квадратичну швидкість збіжності. За обчислювальними витратами на одну ітерацію метод Ньютона можна порівняти з методом зворотної ітерації з відношенням Релея. На відміну від зворотної ітерації, метод Ньютона дозволяє обчислити власну пару з більшою точністю.

Ключові слова: Метод Ньютона, власне значення, симетрична матриця, зворотна ітерація.

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Метод Ньютона для задачи на собственные значения симметричной матрицы

Резюме

Рассмотрен метод Ньютона вычисления собственного значения и соответствующего собственного вектора симметричной вещественной матрицы. Нелинейная система уравнений, решаемая методом Ньютона, состоит из уравнения определяющего собственное значение и собственный вектор матрицы и условия нормировки собственного вектора. Метод позволяет одновременно вычислять собственное значение и соответствующий собственный вектор. Начальные приближения для собственного значения и соответствующего собственного вектора можно найти степенным методом или обратной итерацией со сдвигом. Предложено простое доказательство сходимости метода в окрестности простого собственного значения. Показано, что метод обладает квадратичной скоростью сходимости. По вычислительным затратам на одну итерацию метод Ньютона сравним с методом обратной итерации с отношением Релея. В отличие от обратной итерации, метод Ньютона позволяет вычислять собственную пару с большей точностью.

Ключевые слова: Метод Ньютона, собственное значение, симметричная матрица, обратная итерация.

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