Numerical Method for Eigenvalue Problem and Its Application in Physics

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Abstract

Eigenvalue decomposition of a Hermitian (or real symmetric) matrix is often the last step to solve a physics problem, and thus in this report we investigate different numerical methods for the eigenvalue problem. First two examples, buckling beam problem and quantum dot, are given to illustrate how a differential equation is transformed to an eigenvalue problem of a real symmetric matrix. Then we discuss details of Jacobi's and bisection methods, two important numerical algorithms for the eigenvalue problem. Applications of these two methods on the quantum dot are studied, which shows us when our approximation is good. In addition, we find that bisection method has a better performance and accuracy than Jacobi's. Therefore, bisection algorithm is usually more appropriate to utilize in physics.

1 Introduction

Eigenvalue problem is an important mathematical problem that appears commonly in science and engineering. For matrix $A \in \mathbb{C}^{n\times n}$, its eigenvalues λ_i and corresponding eigenvectors $\mathbf{v}_i \in \mathbb{C}^n$ satisfy

$$A\mathbf{v}_i = \lambda_i \mathbf{v}_i \ . \tag{1}$$

If A is Hermitian (or real symmetric), we can use its eigenvalues and eigenvectors to construct a unitary (or orthogonal) similarity transformation to diagonalize A, i.e.

$$S^\dagger AS = \mathrm{diag}\{\lambda_1, \lambda_2, \cdots, \lambda_n\} \text{ for Hermitian } A \in \mathbb{C}^{n\times n}, \tag{2}$$

$$S^T AS = \mathrm{diag}\{\lambda_1, \lambda_2, \cdots, \lambda_n\} \text{ for symmetric } A \in \mathbb{R}^{n\times n}, \tag{3}$$

where S is a unitary (or orthogonal) matrix and the ith column of S is the eigenvector of A with eigenvalue λ_i.

The diagonalization of a Hermitian (or real symmetric) matrix is usually the final step of a physics problem. In Sec. 2 we give two examples of eigenvalue problems in physics, which shows how a differential equation is transformed to an eigenvalue problem of a real symmetric matrix. Sec. 3 gives two algorithms, Jacobi's method and bisection method, to solve the eigenvalue problem. In Sec. 4 our numerical solutions are compared with the analytical solution to show under what condition our approximation is valid. We also discuss the performance of the two algorithms we implement in Sec. 4. Conclusions and outlook are given in Sec. 5.

2 Examples of eigenvalue problems in physics

2.1 The buckling beam problem

The buckling beam problem involves the following differential equation:

$$\gamma \frac{d^2u(x)}{dx^2} = -Fu(x), \tag{4}$$

where $u(x)$ is the vertical displacement of the beam in y direction. L is the length of the beam, $x \in [0, L]$ and F is a force applied at $(L, 0)$. The parameter γ is a constant defined by the rigidity of the beam. The boundary condition of this problem is set to be $u(0) = u(L) = 0$.

To scale the equation, we define a dimensional variable

$$\rho = \frac{x}{L},$$

and thus $\rho \in [0, 1]$. Eq. 4 becomes

$$\frac{d^2u(\rho)}{d\rho^2} = -\frac{FL^2}{R}u(\rho) = -\lambda u(\rho), \tag{5}$$

with $\lambda = FL^2/R$. The discretized approximation to function u is defined as u_i on $(N + 1)$ equidistant points $\rho_i \in [0, 1]$, where $\rho_0 = 0$ and $\rho_N = 1$. Thus, the grid spacing is $h = 1/N$ and $\rho_i = ih$. Then we approximate the second derivative as

$$u_i'' = u''(\rho_i) = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + O(h^2) \tag{6}$$

And thus Eq. 5 for a given value ρ_i can be rewritten as

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = \lambda u_i. \tag{7}$$

We can rewrite Eq. 7 as an eigenvalue problem:

$$\begin{bmatrix} d & a & 0 & 0 & \dots & 0 & 0 \\ a & d & a & 0 & \dots & 0 & 0 \\ 0 & a & d & a & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & a & d & a \\ 0 & \dots & \dots & \dots & \dots & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}. \tag{8}$$

where $d = 2/h^2$ and $a = -1/h^2$. Endpoints u_0 and u_N are not included in the matrix. This eigenvalue problem has analytical eigenvalues as

$$\lambda_j = d + 2a\cos\left(\frac{j\pi}{N+1}\right) \quad j = 1, 2, \dots N - 1. \tag{9}$$

which will be used for unit tests in Sec. 3.3.

2.2 Quantum dot in three dimensions

The eigenvalue problem commonly appears in quantum mechanics. For illustration, we consider a quantum dot in a three-dimensional harmonic oscillator potential with frequency ω. At first only one electron

is inside the trap and the system is assumed to be spherically symmetric. The radial part of Schrödinger's equation for one electron

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{l(l+1)}{r^2}\right)R(r)+V(r)R(r)=ER(r). \tag{10}$$

where l is the quantum number of orbital angular momentum and $V(r)=\frac{1}{2}m\omega^2r^2$ is the harmonic oscillator potential. The energies of the system is

$$E_{nl}=\hbar\omega\left(2n+l+\frac{3}{2}\right), \tag{11}$$

with $n=0,1,2,\ldots$ and $l=0,1,2,\ldots$ By substituting $R(r)=u(r)/r$ we obtain a more compact form of equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r)+\left(\frac{1}{2}m\omega^2r^2+\frac{l(l+1)}{r^2}\frac{\hbar^2}{2m}\right)u(r)=Eu(r). \tag{12}$$

The boundary conditions are $u(0)=0$ and $u(\infty)=0$.

For simplicity, we only discuss s wave, i.e. $l=0$ case. By defining

$$\alpha=\sqrt{\frac{\hbar}{m\omega}},\quad \rho=\frac{r}{\alpha},$$

Eq. 12 can be written in a simpler form as

$$-\frac{d^2}{d\rho^2}u(\rho)+\rho^2u(\rho)=\lambda u(\rho), \tag{13}$$

with

$$u(\rho=0)=0,\quad u(\rho\to\infty)=0.$$

Here $\lambda=\frac{2E}{\hbar\omega}$ and the centrifugal term disappears as $l=0$. The analytical solutions of λ are $\lambda_0=3,\ \lambda_1=7,\ \lambda_2=11,\ldots$

Since it is impossible to go to infinity when we numerically solve Eq. 13, we choose a maximum radius $\rho_{\max}$ and set $u(\rho_{\max})=0$. Similar to the bulking beam problem discussed in Sec. 2.1, we can define the discretized approximation to function u as u_i on $(N+1)$ equidistant points $\rho_i\in[0,\rho_{\max}]$, where $\rho_0=0$ and $\rho_N=1$. Thus, the grid spacing is $h=1/N$ and $\rho_i=ih$. Then Eq. 13 can be discretized and approximated as

$$-\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}+\rho_i^2u_i=\lambda u_i, \tag{14}$$

where ρ_i^2 comes from the harmonic oscillator potential. Eq. 14 can be rewritten as an eigenvalue problem of a matrix:

$$\begin{bmatrix} d_1 & e_1 & 0 & 0 & \ldots & 0 & 0\\ e_2 & d_2 & e_2 & 0 & \ldots & 0 & 0\\ 0 & e_3 & d_3 & e_3 & 0 & \ldots & 0\\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots\\ 0 & \ldots & \ldots & \ldots & \ldots e_{N-2} & d_{N-2} & e_{N-2}\\ 0 & \ldots & \ldots & \ldots & \ldots & e_{N-1} & d_{N-1}\end{bmatrix}\begin{bmatrix}u_1\\u_2\\\ldots\\\ldots\\\ldots\\u_{N-1}\end{bmatrix}=\lambda\begin{bmatrix}u_1\\u_2\\\ldots\\\ldots\\\ldots\\u_{N-1}\end{bmatrix}. \tag{15}$$

where

$$d_i=\frac{2}{h^2}+\rho_i^2,\quad e_i=-\frac{1}{h^2}. \tag{16}$$

When two electrons are put inside the harmonic oscillator potential, the radial part of Schrödinger's equation can be written as

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2}-\frac{\hbar^2}{4m}\frac{d^2}{dR^2}+\frac{1}{4}m\omega^2r^2+m\omega^2R^2+\frac{\beta e^2}{r}\right)u(r,R)=Eu(r,R). \tag{17}$$

where $\mathbf{R}$ is the center of mass coordinate and $\mathbf{r}$ is the relative coordinate. $\frac{\beta e^2}{r}$ is the Coulomb repulsion between two electrons, with $\beta e^2 = 1.44\ \text{eV}\cdot\text{nm}$. Eq. 17 can be separated into two parts:

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2}+m\omega^2R^2\right)\chi(R)=E_R\chi(R), \tag{18}$$

and

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2}+\frac{1}{4}m\omega^2r^2+\frac{\beta e^2}{r}\right)\psi(r)=E_r\psi(r), \tag{19}$$

where

$$E=E_R+E_r,\quad u(r,R)=\chi(R)\psi(r). \tag{20}$$

Similar to the one-electron case, we define a natural length

$$\alpha'=\frac{\hbar^2}{m\beta e^2}$$

and let $\rho = r/\alpha'$. Then Eq. 19 can be rewritten as

$$-\frac{d^2}{d\rho^2}\psi(\rho)+\omega_r^2\rho^2\psi(\rho)+\frac{1}{\rho}=\lambda\psi(\rho), \tag{21}$$

where

$$\omega_r^2=\frac{m^2\omega^2}{4\hbar^2}\alpha'^4,\quad \lambda=\frac{m\alpha'^2}{\hbar^2}E_r. \tag{22}$$

Similar to Eq. 13, Eq. 21 can be numerically solved by transforming it into an eigenvalue problem

$$\begin{bmatrix} d_1 & e_1 & 0 & 0 & \dots & 0 & 0 \\ e_2 & d_2 & e_2 & 0 & \dots & 0 & 0 \\ 0 & e_3 & d_3 & e_3 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots e_{N-2} & d_{N-2} & e_{N-2} \\ 0 & \dots & \dots & \dots & \dots & e_{N-1} & d_{N-1} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \dots \\ \dots \\ \dots \\ \psi_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} \psi_1 \\ \psi_2 \\ \dots \\ \dots \\ \dots \\ \psi_{N-1} \end{bmatrix}, \tag{23}$$

where

$$d_i=\frac{2}{h^2}+\omega_r^2\rho_i^2+\frac{1}{\rho_i},\quad e_i=-\frac{1}{h^2}. \tag{24}$$

3 Numerical methods

In order to solve the eigenvalue problems that occur naturally in physics, we will investigate two relevant numerical algorithms (Jacobi's method and bisection method) in this section.

3.1 Jacobi's method

Jacobi's method gives a simple algorithm to diagonalize a real symmetric (or Hermitian) matrix. It is based on Givens rotation

$$G(k,l,\theta) = \begin{bmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & c & \cdots & s & \cdots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & -s & \cdots & c & \cdots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix} \tag{25}$$

where $c = \cos\theta$ and $s = \sin\theta$ appear at the intersections of kth and lth rows and columns. Therefore, for $k > l$, non-zero matrix elements of $G(k,l,\theta)$ are given by

$$\begin{aligned} g_{ii} &= 1 \quad \text{if } i \neq k, l \ ; \\ g_{kk} &= g_{ll} = c \ ; \\ g_{kl} &= -g_{lk} = -s \ . \end{aligned}$$

We can see that $G(k,l,\theta)$ is an orthogonal matrix.

Let $A \in \mathbb{R}^{n\times n}$ be symmetric. Our purpose of orthogonal similarity transformation

$$B = G(k,l,\theta)^T A G(k,l,\theta) \tag{26}$$

is to eliminate non-zero off-diagonal elements $a_{kl} = a_{lk}$. To achieve this, we should have $0 = b_{kl} = a_{kl}(c^2 - s^2) + (a_{ll} - a_{kk})cs$, and thus $t = \tan\theta$ should be the solution of

$$t^2 + 2\tau t - 1 = 0 \tag{27}$$

where

$$\tau = \frac{a_{kk} - a_{ll}}{2a_{kl}}. \tag{28}$$

Eq. 27 yields

$$t = -\tau \pm \sqrt{1+\tau^2}. \tag{29}$$

Then c and s can be easily obtained via

$$\begin{aligned} c &= \frac{1}{\sqrt{1+t^2}} \ , \\ s &= tc \ . \end{aligned} \tag{30}$$

Usually we choose the smaller root of Eq. 29, which makes $|\theta| \leq \frac{\pi}{4}$ and minimizes the Frobenius norm [1] of $(B - A)$.

Based on Givens rotation, the main idea of Jacobi's method is to eliminate the off-diagonal element with maximum absolute value by Eq. 25, 26, 29 and 30, until the absolute values of all the off-diagonal elements are less than a specific tolerance. This can also be done in a cyclic way, which avoids the necessity to find the maximum off-diagonal element in each iteration. The pseudocode of Jacobi's method is given in Algorithm 1.

[1] The Frobenius norm of matrix $A \in \mathbb{C}^{n\times n}$ is defined as

$$||A||_F = \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{n} |a_{ij}|^2} \ .$$

It is conserved in unitary (or orthogonal) similarity transformation.

Input: Symmetric matrix $A \in \mathbb{R}^{n \times n}$, tolerance and maxiter.
Output: Eigenvalues in vector **u** and corresponding eigenvectors in columns of matrix $S \in \mathbb{R}^{n \times n}$.

S=identity matrix;
while maxnondiag > tolerance && iterations <= maxiter **do**
  iterations++;
  Find the maximum non-diagonal element a_{kl} $(k > l)$ in matrix A;
  Calculate t, c and s via Eq. 29 and 30 and obtain $G(k, l, \theta)$;
  $A = G(k, l, \theta)^T A G(k, l, \theta)$ (Eq. 26);
  $S = SG(k, l, \theta)$;
end
for $i = 1; i <= n; i++$ **do**
  $u_i = a_{ii}$;
end
return **u**,S;

Algorithm 1: Jacobi's method for diagonalization of symmetric matrix $A \in \mathbb{R}^{n \times n}$.

3.2 Bisection method

Wait to be filled by Mengzhi.

3.3 Unit tests for development

As is stated in Sec. 2.1, the eigenvalue problem of Eq. 8 has an analytical expression (Eq. 9). Therefore, we employ Eq. 9 to construct a unit test for our eigenvalue solvers during the development, which is done with the help of Catch2 library. In addition, the conservation of Frobenius norm and the orthogonality of eigenvectors are also tested to confirm the correctness of our codes.

4 Results and discussion

4.1 Results of the quantum dot problem

In this section we discuss the results of quantum dot obtained from Jacobi's method (Sec. 3.1) with different $\rho_{\max}$ and grid points N. Tolerance of the maximum off-diagonal element is 10^{-5}.

4.2 Performance comparison of different methods

Wait to be filled by Mengzhi.

5 Conclusions and outlook

Wait to be filled.

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References

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