Numerical Method for Eigenvalue Problem and Its Application in Physics

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Abstract

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1 Introduction

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2 Examples of eigenvalue problems in physics

2.1 The buckling beam problem

The buckling beam problem involves the following differential equation:

$$\gamma \frac{d^2u(x)}{dx^2} = -Fu(x), \tag{1}$$

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. 1 becomes

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

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

$$u_i'' = u''(\rho_i) = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + O(h^2) \tag{3}$$

And thus Eq. 2 for a given value ρ_i can be rewritten as

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = \lambda u_i. \tag{4}$$

We can rewrite Eq. 4 as an eigenvalue problem:

$$\begin{bmatrix} d & a & 0 & 0 & \dots & 0 & 0 \\ a & d & a & 0 & \dots & 0 & 0 \\ 0 & a & d & a & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & a & d & a \\ 0 & \dots & \dots & \dots & \dots & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}. \tag{5}$$

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

$$\lambda_j = d + 2a\cos\left(\frac{j\pi}{N+1}\right) \quad j = 1, 2, \dots N-1. \tag{6}$$

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

2.2 Quantum dots in three dimensions

The eigenvalue problem commonly appears in quantum mechanics. For illustration, we consider quantum dots 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

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)R(r) + V(r)R(r) = ER(r). \tag{7}$$

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

$$E_{nl} = \hbar\omega\left(2n + l + \frac{3}{2}\right), \tag{8}$$

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

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + \left(\frac{1}{2}m\omega^2 r^2 + \frac{l(l+1)}{r^2}\frac{\hbar^2}{2m}\right)u(r) = Eu(r). \tag{9}$$

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. 9 can be written in a simpler form as

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2 u(\rho) = \lambda u(\rho), \tag{10}$$

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 $\lambda_0 = 3,\ \lambda_1 = 7,\ \lambda_2 = 11, \dots$

Since it is impossible to go to infinity when we numerically solve Eq. 10, 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. 10 can be discretized and approximated as

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \rho_i^2 u_i = \lambda u_i, \tag{11}$$

where ρ_i^2 comes from the harmonic oscillator potential. Eq. 11 can be rewritten as an eigenvalue problem of a matrix:

$$\begin{bmatrix} d_1 & e_1 & 0 & 0 & \dots & 0 & 0 \\ e_2 & d_2 & e_2 & 0 & \dots & 0 & 0 \\ 0 & e_3 & d_3 & e_3 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots e_{N-2} & d_{N-2} & e_{N-2} \\ 0 & \dots & \dots & \dots & \dots & e_{N-1} & d_{N-1} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_{N-1} \end{bmatrix}. \tag{12}$$

where

$$d_i = \frac{2}{h^2} + \rho_i^2, \quad e_i = -\frac{1}{h^2}. \tag{13}$$

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

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} - \frac{\hbar^2}{4m}\frac{d^2}{dR^2} + \frac{1}{4}m\omega^2 r^2 + m\omega^2 R^2 + \frac{\beta e^2}{r}\right) u(r, R) = E u(r, R). \tag{14}$$

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. 14 can be separated into two parts:

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + m\omega^2 R^2\right) \chi(R) = E_R \chi(R), \tag{15}$$

and

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{1}{4}m\omega^2 r^2 + \frac{\beta e^2}{r}\right) \psi(r) = E_r \psi(r), \tag{16}$$

where

$$E = E_R + E_r, \quad u(r, R) = \chi(R)\psi(r). \tag{17}$$

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. 16 can be rewritten as

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2 \rho^2 \psi(\rho) + \frac{1}{\rho} = \lambda \psi(\rho), \tag{18}$$

where

$$\omega_r^2 = \frac{m^2\omega^2}{4\hbar^2}\alpha'^4, \quad \lambda = \frac{m\alpha'^2}{\hbar^2}E_r. \tag{19}$$

Similar to Eq. 10, Eq. 18 can be numerically solved by transforming it into an eigenvalue problem

$$\begin{bmatrix} d_1 & e_1 & 0 & 0 & \dots & 0 & 0 \\ e_2 & d_2 & e_2 & 0 & \dots & 0 & 0 \\ 0 & e_3 & d_3 & e_3 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots e_{N-2} & d_{N-2} & e_{N-2} \\ 0 & \dots & \dots & \dots & \dots & e_{N-1} & d_{N-1} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \dots \\ \dots \\ \dots \\ \psi_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} \psi_1 \\ \psi_2 \\ \dots \\ \dots \\ \dots \\ \psi_{N-1} \end{bmatrix}, \tag{20}$$

where

$$d_i = \frac{2}{h^2} + \omega_r^2 \rho_i^2 + \frac{1}{\rho_i}, \quad e_i = -\frac{1}{h^2}. \tag{21}$$

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

$$G(k,l,\theta) = \begin{bmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & c & \cdots & s & \cdots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & -s & \cdots & c & \cdots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix} \tag{22}$$

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

$$B = G(k,l,\theta)^T A G(k,l,\theta) \tag{23}$$

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

$$t^2 + 2\tau t - 1 = 0 \tag{24}$$

where

$$\tau = \frac{a_{kk} - a_{ll}}{2a_{kl}}. \tag{25}$$

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. 26 and 27 and obtain $G(k, l, \theta)$;
  $A = G(k, l, \theta)^T AG(k, l, \theta)$ (Eq. 23);
  $S = SG(k, l, \theta)$;
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 $A \in \mathbb{R}^{n\times n}$.

Eq. 24 yields

$$t = -\tau \pm \sqrt{1 + \tau^2}. \tag{26}$$

Then c and s can be easily obtained via

$$\begin{aligned} c &= \frac{1}{\sqrt{1+t^2}}\ , \\ s &= tc\ . \end{aligned} \tag{27}$$

Usually we choose the smaller root of Eq. 26, which makes $|\theta| \leq \frac{\pi}{4}$ and minimize 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. 22, 23, 26 and 27, until the absolute values of all the off-diagonal elements are less than a specific tolerance. The pseudocode of Jacobi's method is given in Algorithm 1.

3.2 Bisection method

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3.3 Unit tests for development

As is stated in Sec. 2.1, the eigenvalue problem of Eq. 5 has an analytical expression (Eq. 6). Therefore, we employ Eq. 6 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.

[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.

4 Results and discussion

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5 Conclusions and outlook

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