Methods of solving eigenvalue problems

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Abstract

1 Introduction

A great variety of problems in the physical sciences can be represented as eigenvalue problems, which generally takes the form:

$$O\mathbf{v} = \lambda\mathbf{v}, \tag{1}$$

where O is an operator, λ is an eigenvalue, and $\mathbf{v}$ is an eigenvector. Such problems can easily be solved in terms of linear algebra, and is therefore of great use in simplifying complicated problems, as well as providing a framework for creating efficient algorithms. In particular, we will look at the motion of a fixed buckling beam, and show that this is numerically identical to the motion of quantum dots. Specifically, we will solve following eigenvalue problem

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}v(x) = \lambda v(x). \tag{2}$$

Starting with the methods section, we will present the buckling beam problem, as well as the quantum dot problem, scaling and generalising them to the form of eq. 1. Using different numerical methods, we will use unit testing to make sure that each algorithm is implemented correctly. Moving on to the results section, we will present the efficiency and error of each algorithm in terms of CPU-time and relative error respectively. Then finally, in the discussion section, we will compare the different methods, and look at more possiblities for problems that can be solved using the same general algorithms.

2 Methods

2.1 The buckling beam

Considering first the buckling beam problem, we have

$$\gamma\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = -Fu(x), \quad x \in [0, L] \tag{3}$$

where γ is a property constant, $u(x)$ the vertical displacement, and F the force applied at (L, 0) towards the origin. We can scale this equation by defining a parameter $\rho = \frac{x}{L}$. Inserting, we get

$$-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}u(\rho) = \lambda u(\rho), \quad \rho \in [0, 1] \tag{4}$$

where $\lambda = \frac{FL^2}{\gamma}$. Now we see that this equation is on the form of eq. 2. However, enforcing Dirichlet boundary conditions $u(0) = u(1) = 0$ and using a 2nd order central approximation for n integration steps:

$$\frac{v_{i+1} - 2v_i + v_{i-1}}{h^2} + \mathcal{O}\big(h^2\big) = \lambda_i v_i, \tag{5}$$

where $h = \frac{1}{n+1}$. Disregarding the boundaries (which are set to 0) we obtain the eigenvalue equations

$$A\mathbf{v} = \lambda\mathbf{v}. \tag{6}$$

Here

$$A = \begin{bmatrix} d & a & 0 & \dots & \dots & 0 \\ a & d & a & 0 & \dots & 0 \\ 0 & a & d & a & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \ddots & a & d & a \\ 0 & \dots & \dots & 0 & a & d \end{bmatrix}, \quad (7)$$

is an tridiagonal matrix where $d = \frac{2}{h^2}$ and $a = -\frac{1}{h^2}$, λ is an eigenvalue, and $\mathbf{v} \in (0, n)$ is an eigenvector. The analytical eigenvalues are given by

$$\lambda_j = d + 2a\cos\left(\frac{j\pi}{n+1}\right), \quad (8)$$

$j = 1, 2, \dots n-1$.

2.2 Quantum dots

We want to model an electron in a three dimensional harmonic oscillator potential

$$V(r) = \frac{1}{2}m\omega^2 r^2, \quad r = \sqrt{x^2 + y^2 + z^2} \quad (9)$$

$r \in (0, \infty)$, m is the mass, and ω is the frequency. The quantum state can then be represented as the wavefunction

$$|\Psi\rangle \simeq \Psi(r, \phi, \theta) = R(r)Y_l^m(\phi, \theta), \quad (10)$$

where $R(r)$ is the radial part, and $Y_l^m(\theta, \phi)$ are the spherical harmonics. For reasons that will be elaborated further later, what we need to solve then is the radial equation (see appendix for more details on the wavefunction and the radial eq.)

$$-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - V(r) - \frac{l(l+1)}{r^2}\right)u(r) = Eu(r). \quad (11)$$

Here l is the orbital momentum, $u(r) = rR(r)$, and E are the eigenvalues of $\Psi(r, \theta, \phi)$. We will assume our electron has no orbital momentum ($l = 0$), and scale eq. 11 by substituting $\rho = \frac{r}{\alpha}$ and $\lambda = \frac{E}{\epsilon}$, inserting $V(r)$, and get

$$-\frac{\hbar^2}{2m\alpha^2}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{m^2\omega^2\alpha^4}{\hbar^2}\rho^2\right)u(\rho) = \epsilon\lambda u(\rho), \quad (12)$$

where we can define a natural energy scale $\epsilon = \frac{\hbar^2}{2m\alpha^2}$, and a natural length scale $\alpha = \sqrt{\frac{\hbar}{m\omega}}$, yielding the dimensionless equation

$$-\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} + \rho^2 u(\rho) = \lambda u(\rho). \quad (13)$$

Discretising as in eq. 5, the equation becomes

$$-\frac{v_{i+1} - 2v_i + v_{i-1}}{h^2} + V_i v_i = \lambda v_i, \quad (14)$$

where $V_i = \rho_i^2 = (ih)^2$. Enforcing the Dirichlet boundary conditions, we see that 14 can be written on the same form as 6

$$A\mathbf{v} = \lambda\mathbf{v}. \quad (15)$$

Here

$$A = \begin{bmatrix} \widetilde{d}_1 & a & 0 & \dots & \dots & 0 \\ a & \widetilde{d}_2 & a & 0 & \dots & 0 \\ 0 & a & \widetilde{d}_3 & a & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \ddots & a & \widetilde{d}_{n-1} & a \\ 0 & \dots & \dots & 0 & a & \widetilde{d}_n \end{bmatrix}, \quad (16)$$

where $\widetilde{d}_i = \frac{2}{h^2} + V_i$ and a is as before.

2.3 Algorithm: Jacobi's determinant

2.4 Programming technicalities

3 Results

4 Discussion

$\mathbf{n}$	$\mathbf{t_g/t_s}$	$\mathbf{t_{LU}/t_s}$
10	2.08	3.70
10^2	1.89	$1.00 \cdot 10^2$
10^3	1.48	$1.05 \cdot 10^4$
10^4	1.43	$1.18 \cdot 10^6$
10^5	1.39	-
10^6	1.41	-
10^7	1.39	-

Table 1: Ratio between CPU time for the general algorithm ($\mathbf{t_g}$), the special algorithm ($\mathbf{t_g}$) and the LU decomposition algorithm ($\mathbf{t_{LU}}$) for different matrix sizes ($\mathbf{n}$). The LU decomposition crashed for $\mathbf{n}$ greater than 10^4.

A

$$examplematrix = \begin{bmatrix} b_1 & c_1 & 0 & \dots & \dots & 0 \\ a_1 & b_2 & c_2 & 0 & \dots & 0 \\ 0 & a_2 & b_3 & c_3 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \ddots & a_{n-2} & b_{n-1} & c_{n-1} \\ 0 & \dots & \dots & 0 & a_{n-1} & b_n \end{bmatrix},$$

Figure 1: The numeric solution using different solving algorithms. The graphs for n=100 and n=1000 are so similar that they are not distinguishable.

Derivation of the radial equation

Considering the case of a particle in a three dimensional harmonic oscillator potential, we have the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r), \quad r = \sqrt{x^2+y^2+z^2} \tag{A.1}$$

which in spherical coordinates is given by

$$H = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V(r) + \frac{L^2}{2mr^2}, \tag{A.2}$$

where

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right], \tag{A.3}$$

is the squared angular momentum operator. Since L^2 does not act on r, we have that H and L^2 commute, and neglecting spin, a quantum state can then be represented as a wavefunction

$$|\Psi\rangle \simeq \Psi(r,\phi,\theta) = R(r)Y_l^m(\phi,\theta), \tag{A.4}$$

where $R(r)$ is the radial solution, and $Y_l^m(\theta,\phi)$ are the eigenfunctions of L^2 (spherical harmonics). The Schrodinger equation is then

$$HR(r)Y_l^m(\phi,\theta) = ER(r)Y_l^m(\phi,\theta). \tag{A.5}$$

Here E are the eigenvalues of $\Psi(r,\theta,\phi)$. Letting L^2 act on $Y_m^l(\theta,\phi)$ we obtain its eigenvalues $\hbar^2 l(l+1)$. Substituting $R(r) = \frac{u(r)}{r}$, we see that

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\frac{u(r)}{r} = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\left(\frac{\partial u}{\partial r}\frac{1}{r} - \frac{u(r)}{r^2}\right)\right] = \frac{1}{r^2}\left(\frac{\partial u}{\partial r} + r\frac{\partial^2 u}{\partial r^2} - \frac{\partial u}{\partial r}\right) = \frac{1}{r}\frac{\partial^2 u}{\partial r^2}.$$

Multiplying by r on both sides, the problem then reduces to the radial equation

$$-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - V(r) - \frac{l(l+1)}{r^2}\right)u(r) = Eu(r). \tag{A.6}$$