FYS3150-Project 2

Marcus Berget, Sebastian Amundsen, Andreas Wetzel

August 2020

Abstract

1 Introduction

The aim of this project is solving eigenvalue/eigenvector problems using the Jacobi algorithm. Specifically, we will look at solving the Schroedinger's equation with a three-dimensional harmonic oscillator potential. We will look at how a quantum mechanics problem can be solved as a diagonalization problem.

2 Theory

We will look at the two point boundary problem of a buckling beam. This problem has analytical solutions, which can be used to check the accuracy of a numerical approximation. The differential equation we wish to solve for the beam of length L is:

$$\gamma \frac{d^2u(x)}{dx^2} = -Fu(x) \qquad x \in [0, L] \tag{1}$$

Where u(x) is the displacement of the beam in the y direction, F is the force applied at (L,0) and γ is a constant. We apply the Dirichlet boundary conditions and set u(0)=u(L)=0. Two of the parameters are known, say F and L. We then set up an eigenvalue problem to find γ. We can rewrite equation 1 as:

$$\gamma \frac{d^2u(\rho)}{dx^2} = -\frac{FL^2}{\gamma}u(\rho) = -\lambda u(\rho) \qquad \rho \in [0, 1] \tag{2}$$

With $\lambda = FL^2/\gamma$, the equation can be solved as an eigenvalue problem.

The first step of solving eigenvalue problems numerically, is of course to set up the matrix. In both the case of solving the buckling beam problem and the quantum mechanical problem the matrix is a tridiagonal matrix. This matrix is given by rewriting the expression for the second derivative of a function u:

$$u'' = \frac{u(p+h) - 2u(p) + u(p-h)}{h^2} + O(h^2)$$

Where $h = \frac{\rho_N - \rho}{N}$ is our step length, $\rho_N = 1$ and $\rho_0 = 0$. This expression can be rewritten as:

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

We can rewrite this equation as an eigenvalue problem:

$$\begin{bmatrix} d & a & 0 & 0 & \dots & 0 & 0 \\ a & d & a & 0 & \dots & 0 & 0 \\ 0 & a & d & a & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & a & d & a \\ 0 & \dots & \dots & \dots & \dots & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}. \tag{3}$$

The diagonal elements are defined as $d = 2/h^2$ and the non-diagonal elements are defined as $a = -1/h^2$. This eigenvalue problem has analytical eigenpairs, with corresponding eigenvalues:

$$\lambda_j = d + 2a\cos(\frac{j\pi}{N}), \qquad j = 1, 2, \dots N-1.$$

The associated eigenvectors are:

$$\mathbf{u}_j = [\sin(\frac{j\pi}{N}), \sin(\frac{2j\pi}{N}), ..., \sin(\frac{(N-1)j\pi}{N})]^T, \;\; j = 1, 2, \dots N-1.$$

We define $\tan\theta = t = s/c$, where $s = \sin\theta$ and $c = \cos\theta$. We also have:

$$\cot 2\theta = \tau = \frac{a_{ll} - a_{kk}}{2a_{kl}}.$$

We obtain the quadratic equation:

$$t^2 + 2\tau t - 1 = 0,$$

which we use to find t:

$$t = -\tau \pm \sqrt{1+\tau^2},$$

which gives us the variables c and s:

$$c = \frac{1}{\sqrt{1+t^2}},$$

$$s = ct$$

The general expression for the new matrix elements are:

$$b_{ii} = a_{ii}, i \neq k, i \neq l$$

$$b_{ik} = a_{ik}\cos\theta - a_{il}\sin\theta, i \neq k, i \neq l$$
$$b_{il} = a_{il}\cos\theta + a_{ik}\sin\theta, i \neq k, i \neq l$$
$$b_{kk} = a_{kk}\cos^2\theta - 2a_{kl}\cos\theta\sin\theta + a_{ll}\sin^2\theta$$
$$b_{ll} = a_{ll}\cos^2\theta + 2a_{kl}\cos\theta\sin\theta + a_{kk}\sin^2\theta$$
$$b_{kl} = (a_{kk} - a_{ll})\cos\theta\sin\theta + a_{kl}(\cos^2\theta - \sin^2\theta) \tag{4}$$

Where we insert the expressions for c and s.

We will study two electrons in a harmonic oscillator well. The radial Schrödinger equation in this case is:

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} - \frac{\hbar^2}{4m}\frac{d^2}{dR^2} + \frac{1}{4}kr^2 + kR^2\right)u(r,R) = E^{(2)}u(r,R).$$

Were we have introduced the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center-of-mass coordinate $\mathbf{R} = 1/2(\mathbf{r}_1 + \mathbf{r}_2)$. With some manipulation and calculation we arrive at a form which can be solved using the Jacobi method (for calculations and definitions see [1]):

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho} = \lambda\psi(\rho). \tag{5}$$

Where ω_r is a parameter which reflects the strength of the oscillator potential.

3 Method

In the case of the buckling beam problem the matrix becomes very simple, the diagonal elements are all equal (d in equation 3), and the non-diagonal elements are all equal (a in equation 3).

We wish to solve equation 3 by using Jacobi's rotation algorithm. First we find the variables c and s from equation 2 and equation 2. These values are to be implemented in the expression for the new matrix elements given equation 4.

We wish to find out how many similarity transformations we need before all the non-diagonal elements are essentially zero. We wish to illustrate this by plotting the number of Jacobi rotations needed against the dimension of the matrix.

We are also going to compare the eigenvector with the lowest eigenvalue with the analytical solution. We find the analytical eigenvalues by using armadillos functions for diagonalizing a matrix. These values are to be compared with values found using the Jacobi method.

We will solve equation 5 using the values $\omega_r = 0.01$, $\omega_r = 0.5$, $\omega_r = 1$ and $\omega_r = 5$ for the ground state. We will use the same method as we did for the buckling beam. The only difference being that we add the potential $\omega_r^2\rho^2 + 1/\rho$ to the diagonal elements.

4 Implementation

5 Results

6 Discussion

7 Concluding remarks

References

[1] Department of Physics, University of Oslo, Norway, 2020 Project 2 (Computational Physics I FYS3150/FYS4150)