FYS 4150 - Computational Physics
Project 2: Eigenvalue problems

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https://github.com/MetinSa/FYS4150/tree/master/Project_1

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Abstract

This project involves [...]

1. Introduction

The main goal of this project is to develop code for solving eigenvalue problems and use this to study quantum mechanical problems. The project will focus on getting familiar with Jacobi's method, unit testing and scaling equations to obtain dimensionless variables or more convenient variables. First we will study a two-point boundary value problem of a buckling beam or a spring fastened at both sides. Thereafter we will further develop the code by some simple changes to study a harmonic oscillator problem in three dimensions with both one and two electrons. For this problem, we will also study the role of repulsive Coulomb interaction between the electrons.

2. Theoretical background

2.2. **The buckling beam problem.** The motion of a buckling beam with fixed endpoint at the origin and at $x = L$ can be described by the following differential equation

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

Here $u(x)$ is the vertical displacement, F is the force applied at the end of the beam against the origin and γ is a constant defined by the properties of the beam, as for instance the rigidity. The fixed endpoints gives us Dirichlet boundary conditions,

$$u(0) = u(L) = 0.$$

To simplify the problem and make it dimensionless, we can define $\rho = x/L$. Then we get that $\rho \in [0, 1]$. The differential equation then reads

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

where we also have defined $\lambda = FL^2/R$. We know that the second derivative can be approximated as

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

where $h = (\rho_N - \rho_0)/N$ is the step size when we have N steps. ρ_0 is then the first ρ-value and ρ_0 is the last. The ith ρ-value is given by

$$\rho_i = \rho_0 + ih.$$

By defining $u(\rho_i+h) = u_{i+1}$, $u(\rho_i) = u_i$ and $u(\rho_{i-1}) = u_{i-1}$, we get a discretized version of the equation

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

At last, we can use linear algebra to rewrite this to an eigenvalue problem

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

where $d = 2/h^2$ and $a = -1/h^2$. Because we have Dirichlet boundary conditions, the endpoints are excluded. The eigenvalues can be found analytically, and are given by

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

2.2. **Unitary transformations.** If we have an unitary or orthogonal transformation, the orthogonality of the obtained eigenvectors is preserved. This we can show by considering a basis of orthogonal vectors $\mathbf{v}_i$,

$$\mathbf{v}_i = \begin{bmatrix} v_{i1} \\ \vdots \\ v_{in} \end{bmatrix}.$$

Orthogonality gives that

$$\mathbf{v}_j^T \mathbf{v}_i = \delta_{ij}.$$

If we then have an unitary transformation given by $\mathbf{w}_i = \mathbf{U}\mathbf{v}_i$, we get that

$$\mathbf{w}_j^T \mathbf{w}_i = (\mathbf{U}\mathbf{v}_j)^T (\mathbf{U}\mathbf{v}_i) = \mathbf{v}_j^T \mathbf{U}^T \mathbf{U}\mathbf{v}_i.$$

Because the transformation is orthogonal, we know that $\mathbf{U}^T = \mathbf{U}^{-1}$ and $\mathbf{U}^{-1}\mathbf{U} = \mathbf{I}$, where $\mathbf{I}$ is the identity matrix. This gives us further that

$$\mathbf{w}_j^T \mathbf{w}_i = \mathbf{v}_j^T \mathbf{I} \mathbf{v}_i = \mathbf{v}_j^T \mathbf{v}_i = \delta_{ij},$$

which proves that the orthogonality is preserved. Because we know that the dot-product is defined by $\mathbf{v}_j \cdot \mathbf{v}_i = \mathbf{v}_j^T \mathbf{v}_i$, we have aslo proven that the dot-product is preserved.