FYS3150 Project 2

Introduction

The aim of this project can be separated into 3 different parts. The first part is to develop an algorithm for solving general eigenvalue problems, and implement this into code, which can be used to solve a specific problem. The second part is fixated around making sure that the code is running as it should, by using test functions, and to compare it to other algorithms which solves the same problem. The last part is then to transition into physics and see how our numerical methods can be used to study models of physical systems.

Theory

An eigen value problem is defined by the following equation:

$$Ax = \lambda x \tag{1}$$

Where A is a $(n \times n) -$ matrix, x is an unknown eigenvector, and λ is an eigen value. In other words, if you apply a transformation A on a vector you get the same vector back times a constant λ.

Assuming that A is real and symmetric, we can make use of an orthogonal matrix S to find the eigen values. S can be applied such that:

$$S^T AS = D \tag{2}$$

D is a diagonal matrix where each element is an eigen value of A[1]. D is called a similarity transform of A.

An orthogonal matrix has some specific properties. Consider that it consists of S_n vectors. As such:

$$S = [S_1, S_2, \dots, S_n]$$

The first property regards the inner product:

$$\langle S_i, S_j \rangle = \delta_{ij}$$

Where $\delta_{ij} = 1$ when $i = j$, and $\delta_{ij} = 0$ when $i \neq j$.

The second:

$$SS^T = S^T S = S^{-1} S = I$$

The second property can be utilized to show that eigenvalues are preserved after a similarity transformation. If we multiply eq. (1) by S from left side, we get:

$$SAx = \lambda Sx$$

Inserting $I = S^T S$ between A and x will give:

[1] proof is in chapter 8 of: G. Golub, C. Van Loan, Matrix Computations (John Hopkins University Press, 1996)

$$SAS^T(Sx) = \lambda(Sx)$$

As we can see, the eigenvalues are unchanged. However, the eigenvector is changed to Sx, which is important to remember when using similarity transformations.

Jacobi's method

By examining eq. (2) we can see that eigenvalues of A can be found as long as we know matrix S. S is not just any orthogonal matrix. S is a specific matrix which could be hard to find. Jacobi's method is a method where we find multiple orthogonal matrices instead of looking for the exact matrix in one step. With each new transformation we get one step closer to the diagonalized matrix D.

We start by finding the maximum nondiagonal value and use a similarity matrix to make this equal 0. Since the matrix is symmetrical, this can be done on two elements simultaneously. We then apply the transformation $S^T AS = B$, where B is our new matrix that is one step closer to looking like a diagonal matrix. The similarity matrix looks like this:

$$S = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & 0 & \dots \\ 0 & 0 & \dots & \cos\theta & 0 & \dots & 0 & \sin\theta \\ 0 & 0 & \dots & 0 & 1 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & 0 & \dots \\ 0 & 0 & \dots & 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & -\sin\theta & \dots & \dots & 0 & \cos\theta \end{pmatrix}$$

The matrix elements along the diagonal are all 1, except for $s_{kk} = s_{ll}$ which is $\cos\theta$, and all the nondiagonal elements are 0 except $s_{kl} = -s_{lk} = -\sin\theta$. The k and l is determined by the element which we are going to zero out in matrix A. The similarity transformation can then be described by 6 equations:

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

$$b_{ik} = a_{ik}\cos\theta - a_{il}\sin\theta\,, i \neq k, i \neq l$$

$$b_{il} = a_{il}\cos\theta + a_{ik}\sin\theta\,, i \neq k, i \neq l$$

$$b_{kk} = a_{kk}\cos^2\theta - 2a_{kl}\cos\theta\, sin\theta + a_{ll}\sin^2\theta$$

$$b_{ll} = a_{ll}\cos^2\theta - 2a_{kl}\cos\theta\, sin\theta + a_{kk}\sin^2\theta$$

$$b_{kl} = (a_{kk} - a_{ll})\cos\theta\sin\theta + a_{kl}(\cos^2\theta - \sin^2\theta)$$

We can then let b_{kl} be equal to 0. And divide by $a_{kl}\cos^2\theta$ to get:

$$\frac{a_{kk} - a_{ll}}{a_{kl}}\tan\theta + 1 - \tan^2\theta = 0$$

To clean this up, we can introduce a couple of substitutions:

$$\cos\theta = c, \sin\theta = s, \tan\theta = t, \tau = \frac{a_{kk} - a_{ll}}{2a_{kl}}$$

Which gives us:

$$t^2 + 2\tau t - 1 = 0 \rightarrow t = -\tau \pm \sqrt{1 + \tau^2}$$

Then we can find c and s:

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

Once we have c and s we can finally start to compute the rest of the equations in order to get matrix B.

If you study the equations which are used to find the new elements, you can see that there is a problem that might occur when using Jacobi's method. And that is, for each iteration, we might end up changing the value of elements which are already transformed to 0. The way around this problem is to define a value ϵ that we think is close enough to 0, and then make sure that every nondiagonal element is lower than this value before we stop preforming the transformations.

If we consider an orthogonal basis of vectors v_i:

$$\mathrm{v}_i = \begin{bmatrix} v_{i1} \\ \dots \\ \dots \\ v_{in} \end{bmatrix}$$

Then we know that the unitary transformation U of v_i preserves the orthogonality and dot product.

$$\mathrm{w}_i = \mathrm{U}\mathrm{v}_i \rightarrow \langle \mathrm{w}_i, \mathrm{w}_j \rangle = \langle \mathrm{U}\mathrm{v}_i, \mathrm{U}\mathrm{v}_j \rangle = \mathrm{v}_i^T \mathrm{U}^T \mathrm{U}\mathrm{v}_\mathrm{j} = \mathrm{v}_i^T \mathrm{v}_\mathrm{j} = \delta_{ij}$$

Buckling beam problem

We will now look at how all of this theory can be implemented into physical systems. We start out by taking a look at the buckling beam problem. We have a beam which has length L that is fastened at origin along the x-axis of a coordinate system. There is a force applied to the beam towards the center. The position of the beam in y direction can be described by function $u(x)$, which is given by the following equation:

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

Where $x \in [0, L]$, and $u(0) = u(L) = 0$. γ is a constant which is specific to the material it is made of. We want to define a dimensionless variable that is easier to work with:

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

Where $\rho \in [0,1]$. We can then change the expression to:

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

This is now an eigenvalue problem, which can be solved numerically. We can define the step size as h and the number of steps as N.

$$h = \frac{\rho_N - \rho_0}{N} = \frac{1}{N}$$

u'' can be approximated to the following:

$$u''(\rho_i) \approx \frac{u(\rho_i + h) - 2u(\rho_i) + u(\rho_i - h)}{h^2} = \lambda_i u(\rho_i) \rightarrow -\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = \lambda u_i$$

Which can be rewritten as an eigenvalue problem:

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

Where $d = 2, a = -1$. With analytical solutions:

$$\lambda_j = \frac{2}{h^2} - \frac{2}{h^2}\cos\left(\frac{j\pi}{N}\right), j = 1,2, \dots, N-1$$

$$u_j = \left[\sin\left(\frac{j\pi}{N}\right), \sin\left(\frac{2j\pi}{N}\right), \dots, \sin\left(\frac{(N-1)j\pi}{N}\right)\right]^T, j = 1, 2, \dots, N-1$$

The boundaries are excluded from the eigenvalue problem.

Schrödinger equation for single electron

The problem can be extended to a slightly more complex physical system, which is a single electron in a harmonic oscillator potential. The Schrodinger's equation for this system becomes:

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

Where the potential is equal to $\frac{1}{2}m\omega^2 r^2$ and the energies:

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

Where n and l can be $0, 1, 2, \dots$

Since the potential is not infinite anywhere, the position of the electron could be anywhere.

$r \in [0, \infty)$. We assume that the quantum number l is equal to 0. Then we substitute $R(r)$ with $\frac{1}{r}u(r)$ and introduce a dimensionless variable $\rho = \frac{r}{\alpha}$, where α has dimension length. $V(\rho)$ is then $\frac{1}{2}m\omega^2\alpha^2\rho^2$ or $\frac{1}{2}k\alpha^2\rho^2$, where $k = m\omega^2$. We then end up with:

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\rho^2}u(\rho) + \frac{k}{2}\alpha^2\rho^2 u(\rho) = Eu(\rho)$$

We multiply with $\frac{2m\alpha^2}{\hbar^2}$ on both sides to get:

$$-\frac{d^2}{d\rho^2}u(\rho)+\frac{mk}{\hbar^2}\alpha^4\rho^2u(\rho)=\frac{2m\alpha^2}{\hbar^2}Eu(\rho)$$

By scaling α such that $\frac{mk}{\hbar^2}\alpha^4=1$, and defining $\lambda=\frac{2m\alpha^2}{\hbar^2}$, we finally get:

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

$V(\rho)$ is now simply ρ^2, and our expression looks a lot like the buckling beam expression except for the term $\rho^2u(\rho)$. Discretized, this will look like:

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

Converting this to matrices we get the same as the buckling beam expression:

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

The difference is now that d is equal to $\frac{2}{h^2}+\rho_i^2$. We have to decide what ρ_{max} is in this situation, since we cannot do infinite iterations.

Schrödinger equation for two electrons

We will now look at a system where there are two electrons in a harmonic oscillator, with Coulomb force interactions between the electrons. We start off by temporarily ignoring Coulomb interactions, the Schrödinger equation will then look like:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2}-\frac{\hbar^2}{2m}\frac{d^2}{dr_2^2}+\frac{1}{2}kr_1^2+\frac{1}{2}kr_2^2\right)u(r_1,r_2)=E^{(2)}u(r_1,r_2)$$

This can be expressed with a relative coordinate $r=r_1-r_2$ and the center-of-mass coordinate $R=\frac{1}{2(r_1+r_2)}$. Equation is then:

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

We can separate the function $u(r,R)$ to become $\psi(r)\phi(R)$. The energy $E^{(2)}$ is the sum of E_r and E_R. We are interested in $\psi(r)$, which we can now express as:

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2}+\frac{1}{4}kr^2\right)\psi(r)=E_r\psi(r)$$

Adding the coulomb interaction $V(r)=\frac{\beta e^2}{r}$, we get:

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

Introducing the dimensionless variable ρ once again, and multiplying with $\frac{m\alpha^2}{\hbar^2}$, we get:

$$-\frac{d^2}{d\rho^2}\psi(\rho)+\frac{1}{4}\frac{mk}{\hbar^2}\alpha^4\rho^2\psi(\rho)+\frac{m\alpha\beta e^2}{\rho\hbar^2}\psi(\rho)=\frac{m\alpha^2}{\hbar^2}E_r\psi(\rho)$$

Introducing a new variable:

$$\omega_r^2=\frac{1}{4}\frac{mk}{\hbar^2}\alpha^4$$

And scaling α such that:

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

And defining λ:

$$\lambda=\frac{m\alpha^2}{\hbar^2}E$$

We get the final equation:

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

Which equates to:

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

ω_r is set to 0.01, 0.5, 1 and 5 in the cases we explore.

Results

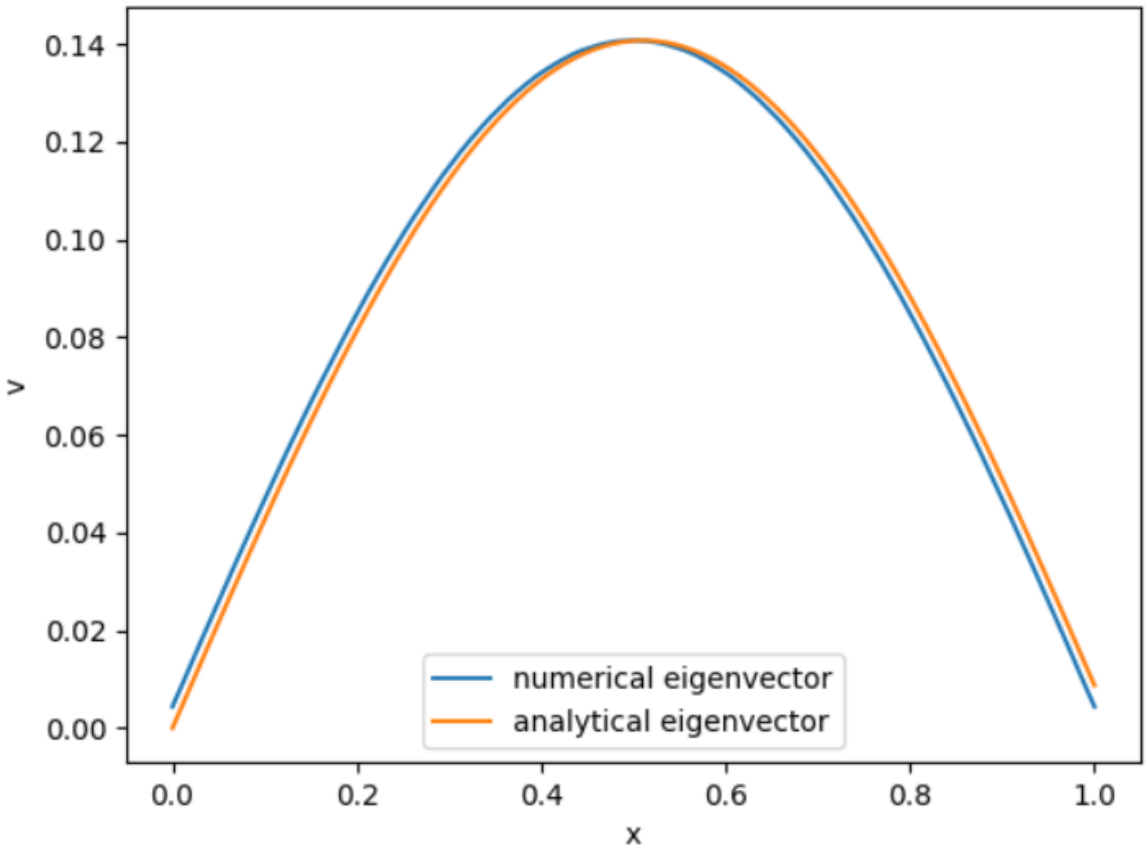

Figure 1: Plot of numerical and analytical eigenvector for the lowest eigenvalue of the buckling beam problem. Both vectors are normalized.