FYS3150 - PROJECT 2
EIGENVALUE PROBLEMS

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Abstract. We present a method for solving eigenvalue problems using similarity transformations, namely the Jacobi rotation method. We show that through dimensional analysis, a problem involving interacting quantum particles can be solved just as easily as a buckling beam problem. We find that Jacobi's method is well suited for problems with low dimensionality, but struggles with higher dimensional ones.

Contents

1. Introduction

A major problem in in computations is dealing with eigenvalue problems. Finding the determinant of a high dimensional matrix by traditional means is extremely computationally heavy, and combined with the fact that there exists no closed form solution to most polynomials of degree five and higher, stated by the Abel-Ruffini theorem, we must find other avenues to solving such problems. We will look at a more computationally friendly algorithm called Jacobi's method, which is a similarity transformation which rotates a matrix around an axis in a hyperplane and transforms it to a diagonal matrix.

2. Theory

2.1. **The Buckling Beam Problem.** We begin by looking at the differential equation for a buckling beam

$$\gamma \frac{d^2u(x)}{dx2} = -Fu(x)$$

This equation solves the vertical displacement $u(x)$ of a beam of length $L, x \in [0, L]$ with a force F applied at $(L, 0)$ towards the origin. The parameter γ is a constant defined by the rigidity and other properties of the beam. Applying a Dirichlet boundary condition we have that $u(0) = u(L) = 0$. In this case the parameters γ, L and F are known. We introduce a new dimentionless variable $\rho = x/L, \rho \in [0, 1]$. The equation can then be reordered to

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

with $\lambda = FL/\gamma$. This is an eigenvalue problem which can be solved by approximating the second derivative as

$$u'' = \frac{u(\rho + h) - 2u(\rho) + u(\rho - h)}{h^2} + O(h^2) \tag{1}$$

where h is the step size. Given a number of n grid points, we can define $h = \frac{\rho_n - \rho_0}{n}$, where $\rho_o = 0$ and $\rho_n = 1$. The value ρ at any point i is then $\rho_i = \rho_0 + ih, i = 1, 2, 3, ..., n$. Rewriting equation 1 in terms of ρ_i it reads

$$-\frac{u(\rho_i + h) - 2u(\rho_i) + u(\rho_i - h)}{h^2} = \lambda u(\rho_i)$$

or in a more compact way

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

Using a matrix representation for this equation it can be written as

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

with $d = 2/h^2$ and $a = -1/h^2$. Since the end points are known, u_0 and u_n are not included.

2.2. **Quantum dots in three dimensions, one electron.** Assuming spherical symmetry, the radial Schrodinger equation for one electron in a harmonic oscillator potential can be written as

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

where $V(r)$ is the harmonic oscillator potential $V(r) = \frac{1}{2}kr^2, k = m\omega^2$ and E is the energy of the harmonic oscillator in three dimensions. The energy levels are defined by

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

where ω is the oscillator frequency, $n = 1, 2, 3, ..$ and the orbital momentum $l = 0, 1, 2, ...$ We will set $l = 0$ since we only are interested in the ground state of the electron. Substituting $R(r) = \frac{1}{r}u(r)$, we obtain

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + V(r)u(r) = Eu(r)$$

Since we have made a transformation to spherical coordinates it means that $r \in [0, \infty)$ and the boundary conditions are $u(0)$ and $u(\infty) = 0$. Our goal here is also to transform the equation to a dimensionless one, so introducing $\rho = \frac{1}{\alpha}r$ where α is a constant with dimension length, and inserting $V(\rho) = \frac{1}{2}k\alpha^2\rho^2$

the equation can be rewritten as

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

By multiplying both sides with $2m\alpha/\hbar^2$ we obtain

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

We fix α so that

$$\frac{mk\alpha^4}{\hbar^2} = 1$$
$$\alpha = \left(\frac{\hbar^2}{mk}\right)^{1/4}$$

and define

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

The Schrodinger equation can then finally be written as

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

By approximating the second derivative of $u(\rho)$ and discretizing our steps and ρ_i by the same method as for the Buckling Beam Problem, the equation can be written compactly as

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

where $V_i = \rho^2$ is the harmonic oscillator potential. Represented in a matrix, it can be written as

$$\begin{bmatrix} d_0 & e_0 & 0 & 0 & \dots & 0 & 0 \\ e_1 & d_1 & e_1 & 0 & \dots & 0 & 0 \\ 0 & e_2 & d_2 & e_2 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots e_{n-1} & d_{n-1} & e_{n-1} \\ 0 & \dots & \dots & \dots & \dots & e_n & d_n \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \dots \\ \dots \\ \dots \\ u_n \end{bmatrix} = \lambda \begin{bmatrix} u_0 \\ u_1 \\ \dots \\ \dots \\ \dots \\ u_n \end{bmatrix}$$

where the diagonal and non-diagonal elements d_i and e_i are

$$d_i = \frac{2}{h^2} + V_i$$
$$e_i = -\frac{1}{h^2}$$

2.3. **Quantum dots in three dimensions, two electrons.** In addition to the harmonic oscillator potential, we will now look at the case where two electrons interact via the repulsive Coulomb force as well. The Schrodinger equation for such a system can be written as

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

The derivation of this formula is done in a similar fashion as the case with just one electron, and can be found in the lecture notes[1] to this course.

2.4. **Unitary transformations of matrices.** By assuming that a matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ is real and symmetric, we know that it must have n eigenvalues $\lambda_1, \lambda_2, .., \lambda_n$. This assumption also implies that there exists a real orthogonal matrix $\mathbf{S}$ such that

$$\mathbf{S^T A S} = diag(\lambda_1, \lambda_2, ..., \lambda_n).$$

We can obtain these eigenvalues of $\mathbf{A}$ by performing a series of similarity transformations, that is

$$\mathbf{B} = \mathbf{S^T A S}, \mathbf{S^T S} = \mathbf{S^{-1} S} = \mathbf{I}$$

The significance of this is that the resulting matrix $\mathbf{B}$ will have the same eigenvalues[2] as $\mathbf{A}$. The obtained eigenvectors will generally not be the same, but their orthogonality, however, will be preserved. To see this, lets consider a basis of vectors $\mathbf{v}_i$, and assume that the basis is orthogonal

$$\mathbf{v_j^T v_i} = \delta_{ij}$$

We perform the unitary transformation $\mathbf{w_i} = \mathbf{U v_i}$ to show that the dot product and orthogonality is preserved

$$\mathbf{w_i^T} = (\mathbf{U v_i})^\mathbf{T} = \mathbf{v_i^T U^T}$$
$$\mathbf{w_i^T w_j} = \mathbf{v_i^T U^T U v_j} = \mathbf{v_i^T v_j} = \delta_{ij}$$

3. Methods

3.1. **Algorithms.** Our general strategy to obtaining the eigenvalues, is to perform a series of similarity transformations on $\mathbf{A}$, as discussed in section 2.4, for the purpose of reducing it to a diagonal form. This will be accomplished by systematically setting the off-diagonal elements of $\mathbf{A}$ to zero by using Jacobi's method.

Consider the following orthogonal transformation matrix

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & 0 & \dots & \dots & \dots & 0 & 0 \\ 0 & 1 & 0 & \ddots & \dots & \dots & 0 & 0 \\ 0 & 0 & \ddots & 0 & \ddots & \dots & 0 & \vdots \\ \vdots & 0 & 0 & \cos\theta & 0 & \ddots & \vdots & \sin\theta \\ \vdots & \vdots & \ddots & 0 & 1 & 0 & \vdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 & \ddots & 0 & \vdots \\ 0 & 0 & \vdots & 0 & \ddots & 0 & 1 & 0 \\ 0 & \dots & 0 & -\sin\theta & 0 & \dots & 0 & \cos\theta \end{bmatrix}$$

Performing the similarity transformation $\mathbf{B} = \mathbf{S^T A S}$, results in

$$\begin{aligned} b_{ik} &= a_{ik}\cos\theta - a_{il}\sin\theta, i \neq k, i \neq l \\ b_{il} &= a_{il}\cos\theta + a_{ik}\sin\theta, i \neq k, i \neq l \\ b_{kk} &= a_{kk}\cos^2\theta - 2a_{kl}\cos\theta\sin\theta + a_{ll}\sin^2\theta \\ b_{ll} &= a_{ll}\cos^2\theta + 2a_{kl}\cos\theta\sin\theta + a_{kk}\sin^2\theta \\ b_{kl} &= (a_{kk} - a_{ll})\cos\theta\sin\theta + a_{kl}\left(\cos^2\theta - \sin^2\theta\right) \end{aligned} \tag{3}$$

Requiring that the off-diagonal elements $b_{kl} = b_{lk}$ are zero, we have that

$$a_{kl}\left(\cos^2\theta - \sin^2\theta\right) + (a_{kk} - a_{ll})\cos\theta\sin\theta = b_{kl} = 0. \tag{4}$$

where $\cos\theta = 1$ and $\sin\theta = 0$ in the event where $a_{kl} = 0$. Further on, we define the quantities

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

equation 4 can be written as

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

which has the roots

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

c and s are then obtained via

$$c = \frac{1}{\sqrt{1 + t^2}} \text{ and } s = tc.$$

With all this in mind, we can implement this method in code by setting up a while loop which runs until all non-diagonal elements of matrix $\mathbf{A}$ are zero within a small tolerance ϵ, which we have set

to $\epsilon = 10^{-10}$.

while $max|a_{ij}| < \epsilon, i \neq j$ **do**
  Choose matrix elements a_{kl} by finding $max|a_{ij}|$;
  if $a_{kl} \neq 0$ **then**
    Compute τ, t, s, c;
  else
    $c = 1$;
    $s = 0$;
  end
  With this set of indices k, l, compute similarity transformation with equations 3, obtaining new matrix $\mathbf{B} = \mathbf{S}(k, l, \theta)^{\mathbf{T}}\mathbf{AS}(k, l, \theta)$;
end

3.2. **Unit tests.** Two test cases have been implemented in code to make sure our program is running as intended. Our first test uses the fact that the buckling beam problem has analytical eigenpairs, with the eigenvalues given as

$$\lambda_j = d + 2a + \cos\big(\frac{j\pi}{N+1}\big), j = 1, 2, 3, ..., N-1$$

where d are the diagonal and a are the off-diagonal matrix elements. The test determines if the results produced by the program are the same as the analytical eigenvalues, within a small $\epsilon = 10^{-5}$, by checking if

$$\sum_{j=1}^{N-1} |\lambda_j^{analytical} - \lambda_j^{computed}| < \epsilon$$

The second test case ensures that our method is capable of finding the largest matrix element a_{ij}. This is done by creating a matrix where we know the indices of the element with the biggest value, and check if the program returns the correct indices.

4. Results

Having a look at the efficiency of the algorithm, we see from figure 4.1 that the number of similarity transformations with respect to the dimensionality of the matrix goes as n^2. The CPU time needed to run the algorithm is shown in figure 4.2. Figure 4.3 shows the ratio between the analytical solutions of the one-particle quantum dots problem and the solutions produced by the Jacobi algorithm. In figure 4.3 we have looked at the ratio between the analytical solutions of the one-particle quantum dots problem with the solutions produced by the Jacobi algorithm, for the four lowest energies. The solutions are quite stable with a dimensionality of 300×300 for $\lambda = 3, 7, 11$, but for higher energy states, the results don't converge to the analytical solution for such small dimensionalities. In the quantum dots problems, we are unable to set $\rho_{max} = \infty$, since ∞ cannot be represented by a computer. We must therefore set this to some finite value. Figure 4.4shows that the solutions quite stable for $\rho_{max} = 5$.
For the quantum dots problem with two interacting electrons in a harmonic oscillator potential, we have plotted the wave function for the lowest energy state. Figure 4.5 shows that the relative distance between the electrons are shorter when the oscillator strength ω_r is stronger, and bigger for a weaker ω_r.

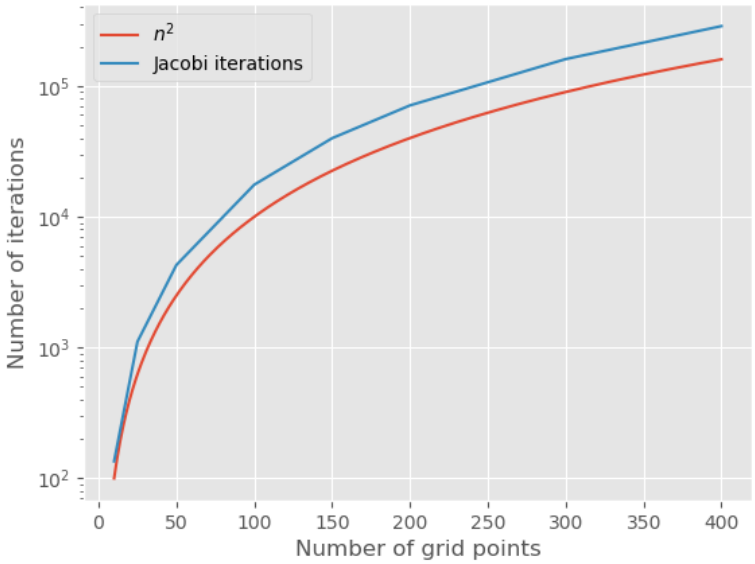

FIGURE 4.1. This plot shows the number of similarity transformations that are needed before all off-diagonal elements are zero, within a tolerance $\epsilon = 10^{-10}$.

5. Conclusion

The fact that we have scaled the equations we have been working with, has demonstrated to be a powerful tool. The systems we have looked at in this project are vastly different in nature, but by using dimensional analysis and scaling, we have been able to implement them in code with only minor differences.

Jacobi's method is a viable option when solving eigenvalue problems with low dimensionality. For systems like the quantum dots, it quickly converges towards the analytical solutions for the lowest energy states. If one is interested in studying for instance higher energy states in quantum systems, our approximation of infinity $\rho_{max} = 5$ would not be sufficient, which leads to having to increase the dimensionality of the problem in order to produce stable results. Another drawback is that we cannot tell how many transformations prior to running the algorithm.

References

[1] Department of Physics, University of Oslo, Norway, Computational Physics FYS3150 Project 2, page 7.
[2] Hjorth-Jensen, M. (2015). Computational Physics, Lecture Notes, page 215.

6. Appendices

Program code for this project can be found on my GitHub.

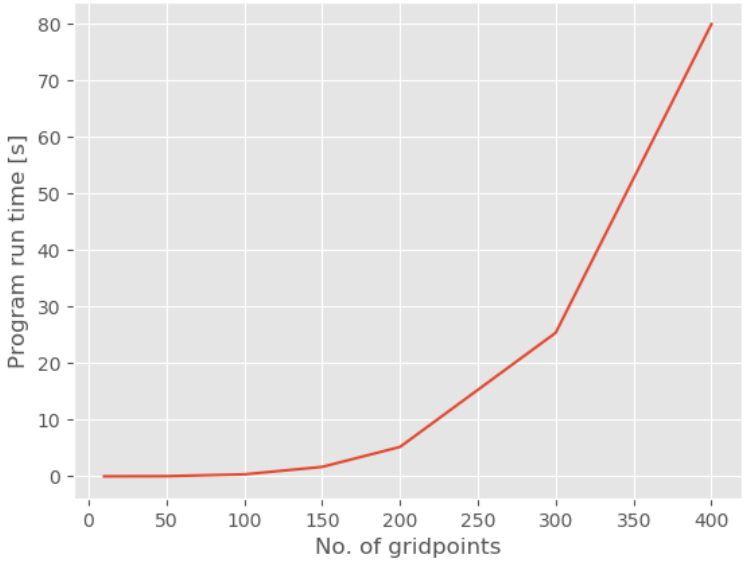

FIGURE 4.2. CPU time for running Jacobi's method with respect to the number of grid points.

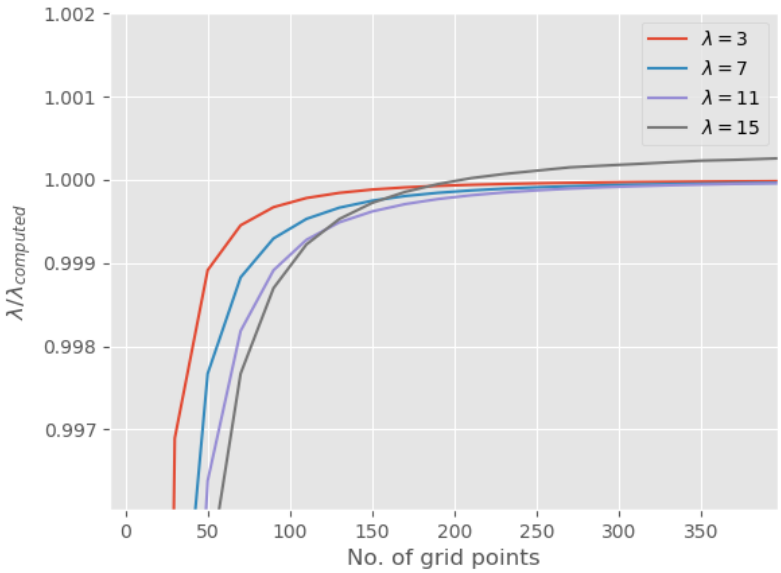

FIGURE 4.3. Convergence towards analytical solutions for the four lowest energy states of the one-particle quantum dots problem.

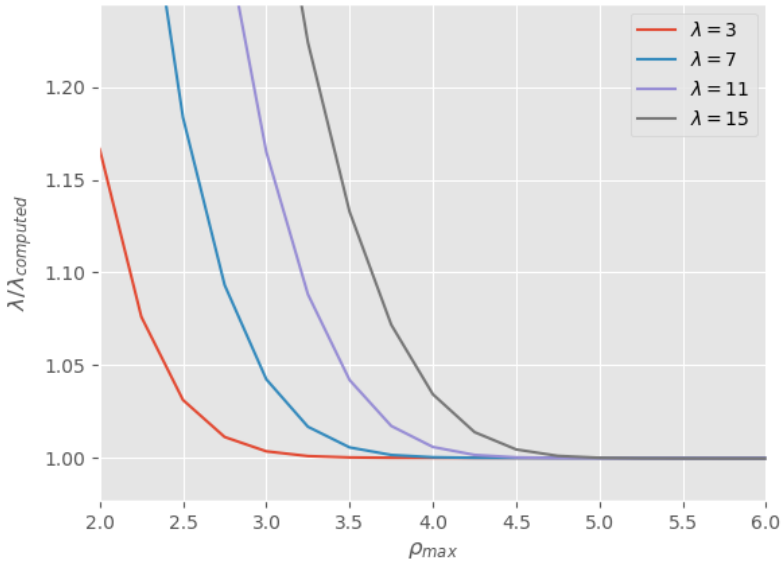

FIGURE 4.4. Convergence towards analytical solutions of the four lowest energy states with different representations of ∞.

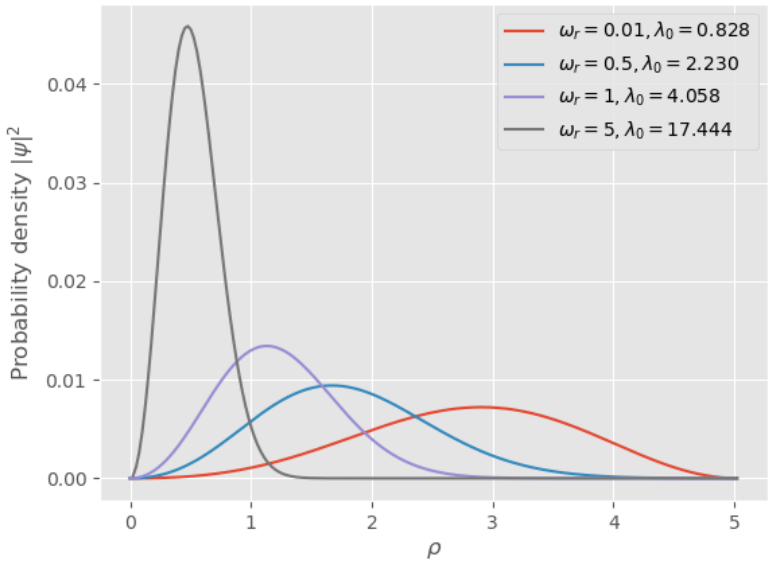

FIGURE 4.5. Relative distance between two electrons in a harmonic oscillator potential, interacting via the repulsive Coulomb force.