# FYS4150 Project 2

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**Abstract**

This project makes use of Jacobi's method for diagonalization on several problems, including the buckling beam, as well as both one and two electrons in a harmonic oscillator potential well. The efficiency of Jacobi's method is investigated, and found to be satisfactory for matrix dimensions up to $n = 400$. Above this, the method proves to be slow and stands no chance against diagonalization methods included in the Armadillo library for C++. In this report, it was found that matrices with dimensions lower than 400 were sufficient to obtain good approximations to analytical eigenvalues for both the buckling beam, as well as the quantum mechanical problems.

## 1 Introduction

Differential equations make up a huge part of physics, mathematics etc. These equations have proven to be excellent representations of a myriad of processes happening in the real world, and that of course brings the complexity of reality to the picture. Differential equations are becoming increasingly hard to solve analytically, if not impossible. Being able to solve these numerically is paramount for our understanding of the universe. In this report, we explore one method for solving such equations, Jacobi's method. We are going to develop an algorithm representing this method and attempt to use it method for solving eigenvalue problems, both representing classical physics as well as the strange world of quantum physics.

# 2 Method

For some beginning mathematics, we will look at a set of basis-vectors.

$$\mathbf{v}_i = \begin{bmatrix} v_{i1} \\ \dots \\ \dots \\ v_{in} \end{bmatrix} \tag{1}$$

Assuming the basis is orthogonal,

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

we will look at a transformation

$$\mathbf{w}_i = \mathbf{U}\mathbf{v}_i.$$

If we say that the transformation is orthogonal, then

$$\mathbf{U}^T\mathbf{U} = \mathbf{U}\mathbf{U}^T = \mathbf{I}.$$

The dot product of the transformation is then

$$\mathbf{w_j^T w_i} = \mathbf{v_j^T U^T U v_i} = \mathbf{v}_j^T \mathbf{v}_i = \delta_{ij},$$

showing that an orthogonal transformation of an orthogonal basis does not change the dot product, nor the orthogonality of the basis.

## 2.1 Buckling beam

We will now look at the buckling beam problem, modeled by differential equation

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

For a beam with length L. $x \in [0, L]$. As we are computational scientists, we would like to solve this numerically. The equation can be rewritten and discretized as

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = \lambda u_i, \tag{3}$$

where $h = \frac{\rho_N - \rho_0}{N}$, $\rho = \frac{x}{L}$, and $\lambda = FL^2/\gamma$. This is now an eigenvalue problem, and can be written into matrix form:

$$\begin{bmatrix} d & a & 0 & 0 & \dots & 0 & 0 \\ a & d & a & 0 & \dots & 0 & 0 \\ 0 & a & d & a & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & a & d & a \\ 0 & \dots & \dots & \dots & \dots & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}. \tag{4}$$

with $d = 2/h^2$ and $a = -1/h^2$. Our aim is to diagonalize this matrix by Jacobi's method and obtain the eigenvalues, analytically given by $\lambda_j = d + 2a\cos(\frac{j\pi}{N+1})$ $j = 1, 2, \ldots N$. We will also investigate the efficiency of this method and compute the number of iterations needed to reach a satisfactory solution, as well as finding the computation time used for different matrix dimensions n.

### 2.2 Quantum dots

We will now add a harmonic oscillator potential $V = \rho^2$ to our matrix diagonal, essentially turning this into a quantum mechanical problem. We will first look at one electron in a harmonic oscillator well, with analytic eigenvalues $\lambda = 3, 7, 11, 15, ...$ Our goal is now to investigate how many integration points needed to make sure our algorithm produces values close to the analytical ones.

Our next step is to add an additional electron to the harmonic oscillator well, giving rise to a repulsive Coulomb interaction. This results in a change of potential $V = \omega_r^2\rho^2 + 1/\rho$, where $\omega_r$ acts as a frequency in our equations. Now, our goal is to obtain the ground state eigenvalues for different $\omega_r$, and compare them to the analytical values given in the article by M. Taut [1].

## 3 Results

### 3.1 Jacobi's method

The number of iterations needed for selected matrix dimensions is shown in table 1. As for the precision of the algorithm, we can compare our new diagonal

| n | Iterations | $1.6n^2$ |
|---|---|---|
| 10 | 146 | 160 |
| 50 | 4058 | 4000 |
| 100 | 16439 | 16000 |
| 200 | 66464 | 64000 |
| 300 | 150261 | 144000 |
| 400 | 268624 | 256000 |

**Table 1:** Table showing the number of iterations needed for diagonalizing a tridiagonal matrix, as a function of matrix dimension n, using Jacobi's method. We see the number of iterations is proportional to $n^2$.

elements with the analytical eigenvalues, shown in table 2.

In table 3, we look at the efficiency of Jacobi's method compared to the eig_sym method included in Armadillo for C++. We see that Jacobi's method is completely outclassed for larger matrices. This is reflected in the amount of iterations needed. This rapid increase in computation speed is likely due to the fact that the method repeatedly overwrites earlier progress by constantly

| Analytical | Diagonal element | Average difference |
|---|---|---|
| 0.0964617 | 0.0965 | |
| 0.36 | 0.36 | |
| 0.72 | 0.72 | 1.67E-16 |
| 1.08 | 1.08 | |
| 1.34354 | 1.3435 | |

**Table 2:** Table showing analytical eigenvalues according to $\lambda_j = d + 2a\cos(\frac{j\pi}{N+1})$ $j = 1, 2, \ldots N$, compared with the diagonal of the diagonalized matrix, dimensionality $n = 5$. The average difference is small enough to show that our algorithm is satisfactory.

assigning new values to the non-diagonals, often larger than previous, in a "two steps forward, one step back" approach.

| n | Armadillo | Jacobi |
|---|---|---|
| 100 | 0.003 s | 0.98 s |
| 200 | 0.013 s | 16.7 s |
| 300 | 0.03 s | 99.5 s |
| 400 | 0.053 s | 450 s |

**Table 3:** Table showing computation times for Jacobi's method and the eig_sym method in Armadillo as a function of matrix dimensionality n. Jacobi's method quickly becomes very slow, while eig_sym is vastly superior.

Regarding the matrix with the added harmonic oscillator potential, table 4 shows how close we are able to approximate the first analytical eigenvalues.

| | n = 100 | n = 200 | n = 300 | n = 400 | $\lambda$ |
|---|---|---|---|---|---|
| Numerical values | 2.99693 | 2.99923 | 2.99966 | 2.99981 | 3 |
| | 6.98465 | 6.99613 | 6.99827 | 6.99903 | 7 |
| | 10.9625 | 10.9906 | 10.9958 | 10.9976 | 11 |
| | 14.9304 | 14.9825 | 14.9922 | 14.9956 | 15 |

**Table 4:** Table comparing numerical eigenvalues with the first analytical eigenvalues $\lambda$ of an electron in a harmonic oscillator potential. The numerical values are obtained by using Jacobi's method on a tridiagonal matrix with added potential. We see the numerical values approaching the analytical ones as the number of integration steps n increases.

### 3.2 Quantum dots

In table 5, we compare our numerical eigenvalues with the eigenvalues for two electrons in a harmonic oscillator well from table I by Taut [1].

| $1/\omega_r$ | Taut | Numerical |
|---|---|---|
| 4 | 0.6250 | 1.2488 |
| 20 | 0.1750 | 0.34996 |
| 54.7386 | 0.0822 | 0.164413 |
| 115.299 | 0.0477 | 0.0954038 |

**Table 5:** Table comparing numerical eigenvalues with tabulated eigenvalues in the article by Taut [1]. Note that Taut's equations have a factor of 1/2, making our ideal values the double of the tabulated ones. We see that our values get closer to the ideal as the frequency $\omega_r$ decreases. A matrix of dimension $n = 200$ was diagonalized with Jacobi's method to obtain our values. $\rho_{max}$ was set to 50.

From the tables, we see the target values being approximated closely and satisfactorily. However, as we tried to increase mesh resolution (read: matrix dimension n) to obtain even better values, the computation times increased greatly as well. If our problem demanded a dimension above 400, say $10^3$ or $10^5$, we would hit a wall where the method would just not be efficient enough to diagonalize the matrices in a reasonable time. Luckily, the problems were designed to make sure we did not have to endure such waiting times. Hopefully in the future, even more efficient methods will be developed to ease our troubled computations and push innovation further.

## 4 Conclusion

Jacobi's method can by all means achieve correct and satisfactory results, and does so in reasonable time, for small matrices. However, therein lies the weakness of the method. It is inefficient and uses brute force, often overwriting earlier progress and needing a great amount of iterations and run time to finish as matrix dimension increases. When the matrices are small however, the method works brilliantly, giving good approximations to the eigenvalues for both buckling beam and harmonic oscillator well problems.

# 5 Appendix

All programs and results can be found here: https://github.com/jensbd/FYS4150/tree/master/Project2

# 6 Bibliography

This report is made possible by lecture slides and code examples in the course, made available by Morten Hjorth-Jensen.

[1] Taut, M., 1993. Two electrons in an external oscillator potential: Particular analytic solutions of a Coulomb correlation problem. Phys. Rev. A 48, 3561–3566. https://doi.org/10.1103/PhysRevA.48.3561

[2] Hjorth-Jensen, M., n.d. Overview of course material: Computational Physics. http://compphysics.github.io/ComputationalPhysics/doc/web/course (accessed 9.7.19).