

# Project 2

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## 1 Abstract

*Main summary of our work - in this project we have ...* Eigenvalue problems, from the equations of a buckling beam to Schroedinger's equation for two electrons in a three-dimensional harmonic oscillator well

## 2 Introduction

*Aims and rationale of the physics case, what you have done - end with brief summary of structure of report* In this project we will solve eigenpair-problems using numerical calculations. We will also implement unit testing in our code to avoid mathematical and programming errors.

We begin by explaining the theoretical models and algorithms we use to compute the eigenvalues, along with technicalities related to the programming of these models.

We will then present and discuss our results, before finally reaching a conclusion regarding the methods we use in terms of efficiency and precision.

## 3 Methods

*Theoretical models and technicalities*

### 3.1 Mathematics

We will start off by proving that orthogonal or unitary transformations preserves the orthogonality/dot product of the vectors.

Starting with an orthogonal basis of vectors,  $\mathbf{v}_i$ , we know that:

$$\mathbf{v}_i = \begin{bmatrix} v_{i1} \\ \vdots \\ v_{in} \end{bmatrix}, \quad \mathbf{v}_j^T \mathbf{v}_i = \delta_{ij}$$

An orthogonal transformation gives us the following:

$$\mathbf{w}_i = U\mathbf{v}_i, \text{ where } U^T U = U U^T = \mathbf{I}$$

We want to prove that orthogonality is preserved:

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

Now that we have proved that orthogonal transformations preserve orthogonality, we can move on to performing our Jacobi iterations. To do so, we use an orthogonal transformation matrix,  $S$ :

$$S = \begin{bmatrix} 1 & 0 & \cdots & & \\ 0 & 1 & 0 & & \\ \vdots & 0 & \ddots & & \\ & \cos \theta & 0 & \cdots & \sin \theta \\ & 0 & 1 & \cdots & 0 \\ & \vdots & \vdots & \ddots & \vdots \\ & -\sin \theta & 0 & \cdots & \cos \theta \end{bmatrix}, \quad S^T = S^{-1}$$

We simplify by assigning:

$$c = \cos \theta, s = \sin \theta, t = \tan \theta = \frac{s}{c}$$

For our positive definite matrix  $A$ , we perform the transformation  $S^T A S = B$ , giving us the general expression:

$$\begin{aligned} b_{ii} &= a_{ii}, i \neq k, i \neq l \\ b_{ik} &= a_{ik}c - a_{il}s, i \neq k, i \neq l \\ b_{il} &= a_{il}c + a_{ik}s, i \neq k, i \neq l \\ b_{kk} &= a_{kk}c^2 - 2a_{kl}cs + a_{ll}s^2 \\ b_{ll} &= a_{ll}c^2 - 2a_{kl}cs + a_{kk}s^2 \\ b_{kl} &= (a_{kk} - a_{ll})cs + a_{kl}(c^2 - s^2) \end{aligned}$$

By choosing the largest non-diagonal element in the original matrix  $A$ , we can fix  $\theta$  by choosing to set the largest non-diagonal element to zero. From this, we can deduce the required values of  $c$  and  $s$ :

$$\begin{aligned} c &= \frac{1}{\sqrt{1+t^2}}, \quad s = tc \\ t &= -\tau \pm \sqrt{1+\tau^2}, \quad \tau = \frac{a_{ll} - a_{kk}}{2a_{kl}} \end{aligned}$$

This will result in a new matrix,  $B$ . We can then find the largest non-diagonal element of the new matrix and repeat the algorithm until this value is less than a given tolerance.

$$B_2 = S_2^T B S_2$$

When this is achieved, we will have a diagonal matrix, where all non-diagonal matrix elements are approaching 0.

$$D = S_n^T S_{n-1}^T \cdots S_1^T A S_1 \cdots S_{n-1} S_n$$

Since we have only performed orthogonal transformations, the eigenvalues for  $D$  and  $A$  will be the same. Since diagonal matrices have their eigenvalues on the diagonal, we can easily read off the eigenvalues.

### 3.1.1 Quantum dots in three dimensions, one electron

We will now consider a physical application of our algorithm by adapting it in order to solve the three dimensional Schrödinger Equation. The general radial form of this equation is:

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

We can now do a series of substitutions and insert some boundary conditions. We assume  $l = 0$ .

$$R(r) = \frac{1}{r} u(r), \quad u(0) = u(\infty) = 0$$

$$\rho = \frac{1}{\alpha} r$$

$$V(\rho) = \frac{1}{2} k \alpha^2 \rho^2$$

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

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

We can then rewrite the Schrödinger Equation like this:

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

We can now discretise this equation by defining the step length  $h$  and  $\rho_{min} = \rho_0$ . We also need to approximate  $\infty$ , as the computer cannot represent infinity:  $\rho_{max} = \rho_N$ .

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

$$\rho_i = \rho_0 + ih, \quad i = 1, \dots, N$$

The Schrödinger equation now becomes:

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

Where  $u_i = u(\rho_i)$  and  $u_{i\pm 1} = u(\rho_i) \pm h$  and  $V_i = \rho_i^2$ . We can then see that the Schrödinger equation can be simplified even more:

$$\begin{aligned} d_i u_i + e_i u_{i-1} + e_i u_{i+1} &= \lambda u_i \\ d_i &= \frac{2}{h^2} + V_i \\ e_i &= -\frac{1}{h^2} = e \end{aligned}$$

Where  $d_i$  are the diagonal elements of our tridiagonal matrix, and  $e_i$  are the non-diagonal elements, which are all equal. This lets us rewrite the Schrödinger equation as a linear problem:

$$\begin{bmatrix} d_1 & e & 0 & 0 & \dots & 0 & 0 \\ e & d_2 & e & 0 & \dots & 0 & 0 \\ 0 & e & d_3 & e & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots e & d_{N-2} & e \\ 0 & \dots & \dots & \dots & \dots & e & d_{N-1} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_{N-1} \end{bmatrix}$$

We can now see that we can use our algorithm to solve our radial Schrödinger equation. We can then run our algorithms with different number of integration points,  $N$ , and the approximation to  $\infty$ ,  $\rho_{max}$ . The resulting  $\lambda$  values are unitless numbers, which can be transformed back into energies by using the value  $\alpha$ .

### 3.1.2 Quantum dots in three dimensions, two electrons

If we now consider a system with two electrons, the electron repulsion between them will come into play in the Schrödinger equation. By doing a lot of the equivalent substitutions and rewriting the equation, we get to a point where we end up with a linear problem, with a tridiagonal matrix with diagonal elements:

$$d_i = \frac{2}{h^2} + \omega_r^2 \rho^2 + 1/\rho$$

Here,  $\omega_r$  represents the strength of the oscillator potential. We will study the cases  $\omega_r = 0.01, 0.5, 1, 5$ , for the ground state ( $l = 0$ ), and compare these to known analytical solutions of the problem.

## 3.2 Programming

To avoid errors in our code, we implement unit tests at the following points:

\* test \* Test

## 4 Results, discussion

For our eigenproblem-solver, we tested and found a reasonable tolerance,  $10^{-8}$ , so that the algorithm converges without reaching the maximum number of iterations,  $n^3$ . We test this using a tridiagonal matrix:

$$A = \begin{bmatrix} 2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & \dots & -1 & 2 \end{bmatrix}$$

Table 1 shows the number of similarity transformations were needed to reach a point where all non-diagonal matrix elements approach 0, for matrix dimensionalities.

Table 1: Dimensionality and number of similarity transformations required to reach the tolerance.

Dimensionality	# of transformations
4	6
10	141
20	551
50	3529

We can see that it looks like  $i = 1.49n^2 - 1.63n - 4.23$ , where  $i$  is number of iterations and  $n$  is dimensionality of the matrix.

Table 2 shows a comparison of eigenvalues found with Armadillo's eigensystem-solver, on our tridiagonal matrix  $A$ .

Table 2: Eigenvalues using the Jacobi method and Armadillo.

$\lambda_{\text{Jacobi}}$	$\lambda_{\text{Armadillo}}$	Diff
0.2679	0.2679	0.0
1.0000	1.0000	0.0
2.0000	2.0000	0.0
3.0000	3.0000	0.0
3.7321	3.7321	0.0

Table 3 shows a comparison of runtimes of the Armadillo eigensystem-solver and our diagonalisation, for a 50x50-matrix.

Table 3: Runtimes using the Jacobi method and Armadillo, for  $n = 50$ .

Jacobi runtime	Armadillo runtime	Diff
0.090051s	0.000405s	0.089646s

#### 4.1 Quantum dots in three dimensions, one electron

Table 4 shows the results of performing our algorithm with the modified diagonal matrix elements of the Schrödinger equation, while varying the number of integration points,  $N$ .

Table 5 shows the result while varying the approximation of  $\rho_{max} = \infty$ . The analytical eigenvalues are:

$$\lambda = 3, 7, 11, 15, \dots$$

Table 4: Numerical eigenvalues, varying  $N$  ( $\rho_{max} = 0.0$ )

$\lambda$	$N$
0.2679	100
1.0000	100
2.0000	100
3.0000	100
0.2679	1000
1.0000	1000
2.0000	1000
3.0000	1000
0.2679	10000
1.0000	10000
2.0000	10000
3.0000	10000

*How many integration points do you need to reproduce analytical results within four leading digits (after the decimal points)?*

#### 4.2 Quantum dots in three dimensions, two electrons

Through trial and error, we determine the ideal  $N = xxxx$  and  $\rho_{max} = 0.9999$ . Varying the strengths of  $\omega_r$ , we get the results in table 6.

*How many integration points do you need to reproduce analytical results within four leading digits (after the decimal points)?*

Table 5: Numerical eigenvalues, varying  $\rho_{max}$  ( $N = 0000$ ).

$\lambda$	$\rho_{max}$
0.2679	5
1.0000	5
2.0000	5
3.0000	5
0.2679	10
1.0000	10
2.0000	10
3.0000	10
0.2679	50
1.0000	50
2.0000	50
3.0000	50

Table 6: Numerical eigenvalues, varying  $\omega_{max}$

$1/\omega_{max}$	$E' = \lambda$
4	0.6250
20	0.1750
54.7386	0.0822
115.299	0.0477

Table 7: Numerical eigenvalues (M. Taut, Phys. Rev. A 48, 3561 (1993)).

$1/\omega_{max}$	$E' = \lambda$
4	0.6250
20	0.1750
54.7386	0.0822
115.299	0.0477

## 5 Conclusions, perspectives

## 6 Appendix, extra material

## 7 Bibliography

M. Taut, Phys. Rev. A 48, 3561 (1993).