3D Quantum Mechanical oscillator with interaction term solved with Jacobi's method
Fys 4150: Project 2

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Abstract

Jacobis method

Introduction

Theory and Algorithms

$$\begin{pmatrix} 2 & -1 & 0 & ... & ... & 0 \\ -1 & 2 & -1 & 0 & ... & 0 \\ 0 & -1 & 2 & -1 & 0 & ... \\ ... & ... & ... & ... & ... & ... \\ 0 & ... & 0 & -1 & 2 & -1 \\ 0 & 0 & ... & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ ... \\ ... \\ u_n \end{pmatrix} = \begin{pmatrix} f_1h^2 \\ f_2h^2 \\ f_3h^2 \\ ... \\ ... \\ f_nh^2 \end{pmatrix} \tag{1}$$

A. Algorithms

Source code and accompanying codes can be found at the git hub address:
https://github.com/ajmarkestad/Fys4150/tree/master/Project2

In this section we want to see how we can employ Jacobi's method with an algorithm that is efficient and fast. We note that as we keep applying transformations until we are somehow close " enough ", given by a measure. It it possible to show that if one chooses[1] to rotate the largest off-diagonal element the Frobenius Norm of the offdiagonal elements will go down in every step. We therefore need to have an efficient algorithm that finds the largest off-diagonal element in an efficient way. We do this with the knowledge that the matrix is symmetric by only looping over the upper-diagonal elements

```
for(int i = 0; i < n; i++){
        for(int j = i+1; j < n; j++){
            if(fabs(A(i,j)) > max){
                max = fabs(A(i,j));
                *l = i;
                *k = j;
            }
        }
    }
```

which gives an $\frac{1}{2}n^2$ scaling with the matrix size. Further Jacobi's method requires a similarity transformation with the matrix S that has 1 on the diagonal except for the places where we want to rotate(for maximum element on element A_{kl} we have $S_{kk} = cos\theta = c = S_{ll}$ and $S_{kl} = sin\theta = s = -S_{lk}$. As explained above we need to calculate s and c to zero out the maximal off-diagonal element, and under this calculation we need to calculate t and τ

$$\tau = \frac{A_{ll} - A_{kk}}{2A_{kl}} \tag{2}$$

$$t = -\tau \pm \sqrt{1 + \tau^2} \tag{3}$$

[1] Lectures Computational Physics FYS3150 UiO

For large values of τ there might be problems in containing the information about the extra $\tau^2 + 1$ as machine precision for float numbers will truncate the 1 if $\tau > 10^9$, leading in the case of subtraction $t = 0$. We want the choose the smallest root as this increases the speed of convergence. Noting our previous problem, we now see that we want to obtain the values where possibly have machine precision problems. That is for positive τ we want to choose the negative root, and need to change the expression by multiplying and dividing by $\tau + \sqrt{1+\tau^2}$. This gives

$$t = \frac{1}{\tau + \sqrt{1+\tau^2}} \tag{4}$$

We then see that for $\tau < 0$ we do the same with $\tau - \sqrt{1+\tau^2}$ leading to

$$t = \frac{-1}{-\tau + \sqrt{1+\tau^2}} \tag{5}$$

Leading to the full algorithm

```
if A(k,l) != 0.00
        tau = (A(l,l) - A(k,k))/(2*A(k,l))
        if tau > 0
                        t = 1.0/(tau + sqrt(1.0 + tau*tau))
        else
                        t = -1.0/(-tau + sqrt(1.0 + tau*tau))
         c = 1/sqrt(1 + t*t)
         s = c*t
else
         c = 1.0
         s = 0.0
```

We then continue to perform the transformation on the columns/rows that are affected. Here we do not perform 2 full matrix multiplications, but carefully only perform the calculations that take place. We see that since the matrix S is almost diagonal except 2 elements, it is possible to show that[2] that only a number of 4n elements needs to be updates for every such rotation. The algorithm shown there is used in our implementation of the Jacobi's method.

Since our matrix is a tridiagonal symmetric matrix, Jacobi's method is not the best algorithm to find eigenvalues and eigenvectors. While it also works on a general dense matrix, we also wanted to test versus a standard library method that is already implemented in armadillo. This is the divide-and-conquer method which should scale in the general case of a dense matrix as $4n^3$ flops[2]. It is rather easy to implement with the following lines

```
mat B = A; //copy for the ARMADILLO solver
vec eigval;
mat eigvec;
eig_sym(eigval, eigvec, B);
```

It is important to note that both methods are not optimised for the tridiagonal case and are meant for dense symmetric matrices. While this might seem like a strange idea, we can use this to see how Jacobi's method performs compared to other state of the art algorithms.

B. Unit-tests

There exist certain mathematical properties that could be exploited to make sure the program and the algorithms run correctly. Since the transformations that occur in the Jacobi's method are either orthogonal or unitary, one can see that the inner product of a given matrix will stay invariant. Under the orthogonal transformation U one has

$$v^T v = v^T U^T U v = (Uv)^T (Uv) = w^T w \tag{6}$$

[2] Computational Physics FYS3150 UiO lecturenotes

while for a unitary transformation W and general complex v

$$v^\dagger v = v^\dagger W^\dagger W v = (Wv)^\dagger (Wv) = w^\dagger w \tag{7}$$

We see that under these transformation the inner product is conserved. We can also check whether orthogonality also is conserved. In the initial basis $\{u_i\}$ the orthogonality relation is $u_j^\dagger u_i = \delta_{ij}$. We transform as earlier

$$\delta_{ij} = u_j^\dagger u_i = u_j^\dagger W^\dagger W u_i = w_j^\dagger w_i \tag{8}$$

which we see has the same property in the transformed system. We can use these identities to construct tests after the Jabobi's method calculation, to ensure that machine error in representing numbers not will perturb the results after running a high number of iterations. We implement this as a unittest for a random, symmetric (10x10) matrix as an initial test of the algorithm and in the end of a run with the full blown set of eigenvectors.

```
//Orthogonality test
for i=0 : n
        for j=0 : n
            innerproduct = dot(vector(i),vector(j))
            if ((i==j) && (abs(abs(innerproduct)-1) > pow(10,-12))) result = "bad";
            if ((i!=j) && (abs(innerproduct)>pow(10,-12))) result = "bad";
        }
    }
```

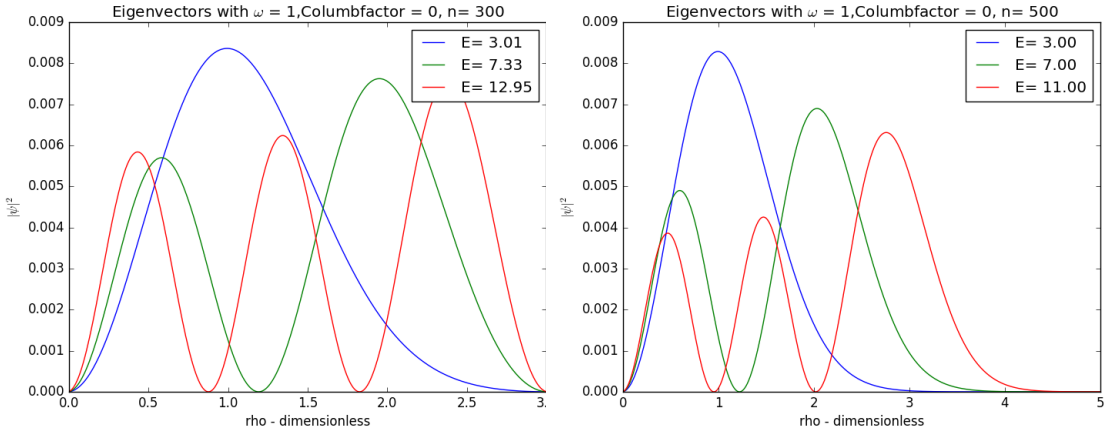
In this setting conserved is a test that the difference is smaller that a given tolerance (in our case $\epsilon = 10^{-12}$). There is also another set of tests that are useful while constructing the programs. These tests rely on simple constructed problems that are solved analytically and compared to the solutions the algorithms give. As we want to find eigenvalues and vectors, we can construct the matrix

$$\begin{pmatrix} 3 & \sqrt{2} \\ 0 & -1 \end{pmatrix}, \quad \lambda_1 = -1, \quad \lambda_2 = 3, \quad v_1 = \begin{pmatrix} -\frac{1}{2\sqrt{2}} \\ 1 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{9}$$

As a solution the program gives -1 and 3 which corresponds perfectly with the analytic solutions. To make sure the subroutines also runs, a test of the functions that finds the maximum off-diagonal element is also included in the startup tests. We initialise a 3x3 empty matrix $\hat{A}$ with the element $A_{1,2} = 1$ to make sure it finds this element, with the correct column and row. For a verification that negative elements function correctly, we also test that on a similar zero-matrix with the element $A_{2,1} = -20, A_{1,2} = 1$ the value -20 is picked out.

Results

The choice of ρ_{max} and the grid size is slightly tricky as we want to make sure we extend the radius long enough to make sure the wavefunction has time to go sufficiently to zero while keeping the spatial resolution high enough not to affect the eigenvalues. From the differential equation with the interaction case it is obvious that for low ω there might be some problems in extending ρ_{max} as the system naturally broadens from the weak oscillator force. In the first test we wanted to make sure we got the same results as the analytical solutions, and were interested in how far we needed to push the grid-size to get 4 digits accuracy. From article (INSERT REFERENCE) we know that the first analytic eigenvalues for $\omega = 1$ and $C_F = 0$ should be 3, 7 and 11. From an arbitrary chosen simulation of 300x300 in figure 1a it is obvious that $\rho_{max} = 3$ gives a too short size for the higher eigenvectors as these in general are pushed further out. Nevertheless we see that for the lowest eigenvalue we get an almost 3 digits correct. We could try to push this up to a higher ρ_{max} but also keeping the relative size of the grids roughly the same. After going up to n=500 and $\rho_{max} = 5$ all the first 4 digits are correct as shown in figure 1b. We suspect that for higher eigenvalues that stretch farther out there is a need for a higher maximal size of the grid together with higher grid sizes for a given precision, and a visual inspection for a general choice of ω and Coulomb Factor to see that all



(a) Harmonic oscillator with grid size = 300, $rho_{max} = 3$, $\omega = 1$ and Columb Factor = 0.

(b) Harmonic oscillator with grid size = 500, $rho_{max} = 5$, $\omega = 1$ and Columb Factor = 0.

Table 1: Energy for the 3 lowest eigenvalues for 4 different potential coefficients

Eigenvalue	λ_1	λ_2	λ_3
$\omega = 0.01$	0.599	0.968	1.347
$\omega = 0.5$	3.001	5.710	8.464
$\omega = 1$	4.058	7.910	11.82
$\omega = 5$	8.323	17.03	25.85

wavefunctions to sufficiently close to zero is a fair method of choosing ρ_{max} and then let the grid size be roughly $\rho_{max} * 100$.

In the general case with no interaction term ($C_F = 0$) we want to see how the strength of the oscillator affects the distribution. We used the recommended values of $\omega = (0.01, 0.5, 1, 5)$. In figure 2a we notice that for a high omega the distribution is pushed towards lower ρ values as the potential gets very steep and the electrons are forces towards the centre of the well. The eigenvalues for the energy for the three lowest states seen in table 1 all increase as the potential increases.

We then focus on the part where we let the interaction term is 1, and want to see how this affects the ground state of the oscillator. To make the results more comparable we use the same range of $\omega = (0.01, 0.5, 1, 5)$ as the previous part. In figure 2b one sees that while including the interaction term the wavefunction gets pushed outwards from the center of mass. Other that this it is important to note that the eigenvalues are substantially higher in this case.

C. Scaling and flops

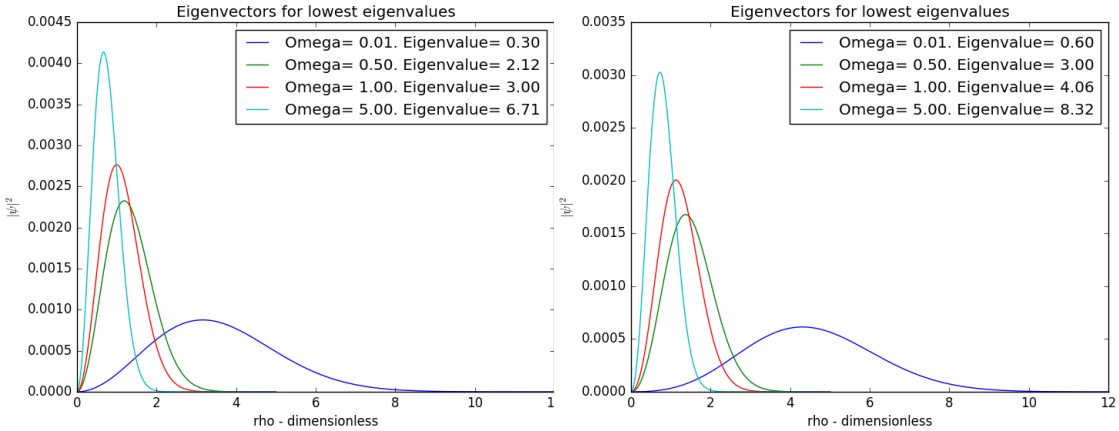
To check the performance and scaling with respect to the grid size, an brute force test that runs the algorithm for different n from 50 to 1000 was performed. Then to find the scaling one approximates the total number of flops with time spend expresses this as a relation which is expected to become more precise for large n

$$T \propto n^a \tag{10}$$

$$log_{10}(T) \approx a \cdot log_{10}(n) \tag{11}$$

In figure 3 one sees that there is a relation between the grid size and the number of operations. After doing a linear regression on the data with equation 11 one finds that

$$T \approx n^{4.0} \tag{12}$$



(a) Eigenstates for the lowest energies with varying harmonic oscillator potential strength $C_F = 0$

(b) Eigenstates for the lowest energies with varying harmonic oscillator potential strength in the interacting case with the $C_F = 1$

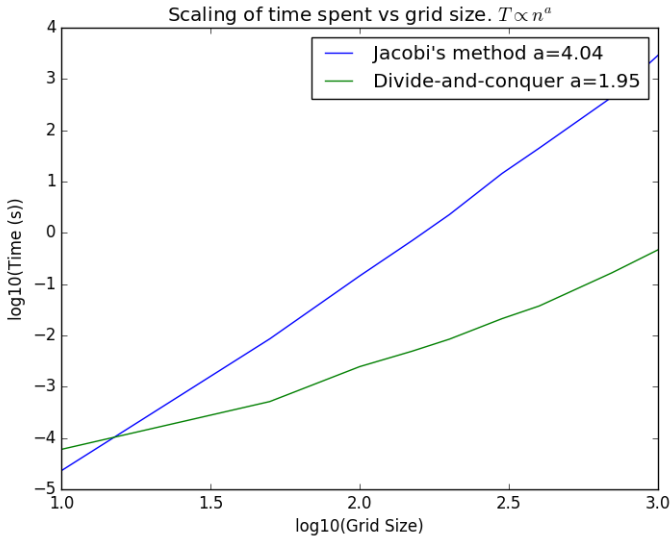


Figure 3: Time spend on finding eigenvalues/vectors for Jacobi's method and the Divide-and-conquer method. This data is from a run on a Macbook Pro 13'

This means that the Jacobi's method scales poorly with increasing grid size. Note that these values are expected to be hardware dependent as the number of operations per second varies with the computer, but the values are nevertheless guiding in evaluating the algorithm. The built in method of divide-and-conquer scales much better and is already faster at $n = 50$. The memory requirements for both methods would also be interesting to study how Jacobi's method does with respect to this dimension as well. From the results of this scaling test we used the armadillo method for $n > 200$ to increase the speed of our calculations as the Jacobi's method simply was to slow in this regime (1 hour for 1000x1000 compared to 0.7 s is a no-brainer).

Conclusion

Jacobi's method is an easy to implement method for finding eigenvalues and eigenvectors for linear algebra problems with symmetric, square matrices up to 1000x1000. Since the scaling behaviour is poor ($time \approx n^4$) for tridiagonal problems, is it not useful as an algorithm for matrices larger that this size. For the numerical experiments with the electrons we see that with these methods get the same dimensionless energy eigenvalues(3,7,11) for the c.o.m part as analytical methods achieve for the non-interacting case, and we can in theory handle arbitrary radial potentials as we could change the input in the program. As expected,

increasing the potential strength ω will keep the particles closer to the center-of-mass and lowering it will give the particles more freedom as they are less confined. When including the interaction term of the type $1/r$ we see that the states are pushed even further out for an arbitrary ω.

References

[1] Morten Hjort-Jensen *Computational Physics Lecture Notes Fall 2015* Department of Physics, University of Oslo 2015 https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Lectures/lectures2015.pdf

[2] Wikipedia: Divide-and-conquer method https://en.wikipedia.org/wiki/Divide-and-conquer_eigenvalue_algorithm