FYS3150 Computational Physics - Project 2

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This is an abstract

INTRODUCTION

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And finally, my implementations of the algorithms discussed in this report can be found on my Github: https://github.com/nicholaskarlsen/FYS3150

THEORY, ALGORITHMS AND METHODS

Preservation of scalar product & orthogonality in unitary transformations

Consider an orthonormal set of basis vectors $\mathbf{v}_i$ such that $\mathbf{v}_j^T\mathbf{v}_i = \delta_{ij}$. Let unitary matrix U where $U^TU = I_N$, where I_N denotes the $N \times N$ identity matrix, operate on $\mathbf{v}_i$ to get $\mathbf{w}_i$

$$\mathbf{w}_i = U\mathbf{v}_i \tag{1}$$

Then

$$\mathbf{w}_j^T\mathbf{w}_i = (U\mathbf{v}_j)^TU\mathbf{v}_i = \mathbf{v}_j^TU^TU\mathbf{v}_i = \mathbf{v}_j^T\mathbf{v}_i = \delta_{ij} \tag{2}$$

In the unitary transformation of $\mathbf{v}_i$ both the scalar product and orthogonality has been preserved.

Givens rotation

A Givens rotation is a unitary transformation which performs a rotation in the plane spanned by two coordinate axes, represented by the matrix in Eqn. 3.

$$G(i,j,\theta) = \begin{bmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \dots & \cos\theta & \dots & -\sin\theta & \dots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \dots & \sin\theta & \dots & \cos\theta & \dots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{bmatrix} \tag{3}$$

where nonzero entries $g_{kk} = 1$ for $k \neq i, j$, $g_{kk} = cos\theta$ for $k = i, j$ and $g_{ji} = -g_{ij} = -\sin\theta$ [2]

As the Givens transformation it unitary, it also follows that it preserves both the scalar product and orthogonality, as shown in the section prior.

Jacobi Eigenvalue Algorithm

The jacobi eigenvalue algorithm finds the eigenpairs of real, symmetric matrices by diagonalization with Givens rotation matrix.

RESULTS AND DISCUSSIONS

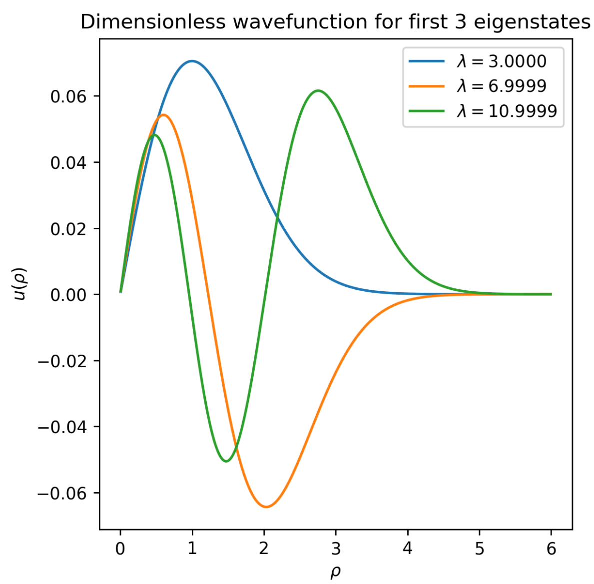

FIG. 1. First 3 eigenpairs in the solution of the harmonic oscillator potential for $N = 1000$, requiring 1386366 transformations.

CONCLUSIONS

[1] M. Hjorth-Jensen, Computational Physics - Lecture Notes 2015, (2015).

[2] Wikipedia contributors, Givens rotation — Wikipedia, The Free Encyclopedia, [Online; accessed 1-October-2018]

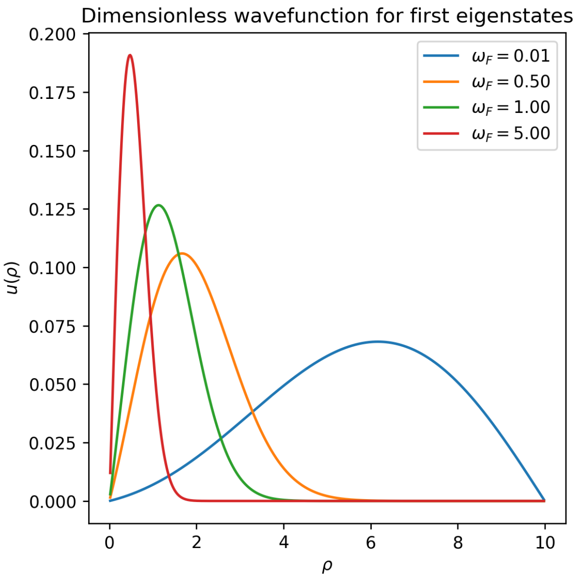

FIG. 2. ...

Jacobi Eigenvalue Algorithm

```
τ = (a_ll − a_kk) / (2 a_kl)

if τ ≥ 0:
        t = 1 / (τ + sqrt(1 + τ^2))
else:
        t = −1 / (−τ + sqrt(1 + τ^2))

c = 1 / sqrt(1 + t^2)
s = tc

a'_kk = a_kk
a'_ll = a_ll

a_kk = c^2 * a'_kk − 2cs * a_kl + s^2 * a'_ll
a_ll = s^2 * a'_kk + 2cs * a_kl + c^2 * a'_ll
a_kl = 0.0
a_lk = 0.0

for  i = 1, 2, ... N:
        if  i ≠ k  and  i ≠ l:
                a_ik = a_ik
                a_il = a_il
                a_ik = c * a_ik − s * a_il
                a_ki = a_ik
                a_il = c * a_il + s * a_ik
                a_li = a_il
```