UNIVERSITY OF OSLO

COMPUTATIONAL PHYSICS

Project 2

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`https://??`

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1 INTRODUCTION

Bla bla bla

The codes written in this project and the results gained from the codes, can be found by following the link: `https://?` to the GitHub repository. [1]

We can ref. to sections etc. using "secref"-command like: Sec. 2

Vectors can be written using "v"-command like: **v**

.... and a lot of other cool stuff!

[1] FiXme Note: correct the these lines

CHAPTER

2 METHOD

Intro to chapter

The source code itself can be found in the GitHub folder `https://??`. [1]

2.1 Nature of the problem

This problem..... bla bla bla.....

2.2 Description of the Algorithm

About the algorithm.....

This is how we write c++ code in the report:

```
// I am a comment

    double please define me;

    for (int i=1 ; i<n ; i++)
    {
        I do this for a lot of i's;
    }
```

2.2.1 Change in Matrix Elements after Iterations and Choice of θ

The algorithm for solving the eigenvalue problem given in [2] contains of multiply similarity transformations of the matrix $\mathbf{A}$, in which we assume a_{kl} to be the largest off-diagonal element. The matrix $\mathbf{B}$ constructed by the similarity transformation is given by

$$\mathbf{B} = \mathbf{S}^T \mathbf{A} \mathbf{S} \tag{2.1}$$

[1] FiXme Note: correct the above lines
[2] FiXme Note: eqref

in which **S** is an orthogonal transformation matrix with its non-zero matrix elements:

$$
\begin{aligned}
s_{kk} &= s_{ll} = \cos\theta \\
s_{kl} &= -s_{lk} = -\sin\theta \\
s_{ii} &= 1, \qquad i \neq k, i \neq l
\end{aligned}
$$

After matrix multiplication with the orthogonal transformation matrix **S** and its transverse (as in (2.1)) the entrances of **B** becomes

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

Due to the symmetry in (2.1) with **A** being a tridiagonal symmetric matrix, $b_{lk} = b_{kl}$, $b_{ki} = b_{ik}$, and $b_{li} = b_{il}$. [3] Since θ can be chosen arbitrarily, we choose θ to be the angle at which b_{kl}, and hence b_{lk}, becomes zero. In this way, the largest element of **A** is eliminated, and it can be shown that this choice of θ reduces the norm of the off-diagonal elements of **A**, which ensures that the algorithm terminates towards the eigenvalues. [4]

This yields the equation

$$0 = (a_{kk} - a_{ll})\cos\theta\sin\theta + a_{kl}(\cos^2\theta - \sin^2\theta) \tag{2.2}$$

By introducing $\tan\theta = \sin\theta/\cos\theta$ and the quantity

$$\tau = \frac{a_{ll} - a_{kk}}{2a_{kl}} \tag{2.3}$$

(2.2) can be rewritten as the quadratic equation in $\tan\theta$

$$\tan^2\theta + 2\tau\tan\theta - 1 = 0 \tag{2.4}$$

which has the solutions

$$\tan\theta = -\tau \pm \sqrt{1+\tau^2} \tag{2.5}$$

From the solutions for $\tan\theta$ given in (2.7), $\cos\theta$ and $\sin\theta$ can be found using the formulas

$$\cos\theta = \frac{1}{\sqrt{1+\tan^2\theta}} \qquad \text{and} \qquad \sin\theta = \tan\theta\cos\theta$$

If $\tau < 0$, $\tan\theta$ is chosen to be

$$\tan\theta = -\tau - \sqrt{1+\tau^2} \tag{2.6}$$

[3] FiXme Note: check that this is actually correct
[4] FiXme Note: this, I can write, right??

whilst if $\tau \geq 0$, $\tan\theta$ is calculated as

$$\tan\theta = -\tau + \sqrt{1+\tau^2} \tag{2.7}$$

This choice is made to always make $\tan\theta$ the smaller of the two roots given in (2.7). Furthermore, this choice ensures that $|\tan\theta| \leq 1$, yielding that $|\theta| \leq \pi/4$.

This is true since $|\tau| \leq 1$, because $|a_{kl}| \geq |a_{ij}|$ for all i, j, from which it follows that

$$|\tan\theta| = \left|-\tau - \sqrt{1+\tau^2}\right| \leq 1, \qquad \text{for } \tau < 0 \tag{2.8}$$

and

$$|\tan\theta| = \left|-\tau + \sqrt{1+\tau^2}\right| \leq 1, \qquad \text{for } \tau \geq 0 \tag{2.9}$$

since $\sqrt{1+\tau^2} \leq \sqrt{2}$.

The fact that $|\theta| \leq \pi/4$ ensures that $\cos\theta \geq 0$ which ultimately ensures that the difference between $\mathbf{A}$ and the new matrix $\mathbf{B}$ is minimized, since

$$||\mathbf{B}-\mathbf{A}||_F^2 = 4(1-c)\sum_{i=1,i\neq k,l}^{n}(a_{ik}^2 + a_{il}^2) + \frac{2a_{kl}^2}{c^2}. \tag{2.10}$$

[5]

[5] FiXme Note: and why is this minimization a good thing?? :-P

CHAPTER

3 RESULTS

When running the code presented in Chap. 2.... blah blah blah.... Let's have an intro to this chapter...

The results from running the code ... can be found in the GitHub folder `https://??`. [1]

3.1 Interpretation of Results

WOW, an awesome interpretation of the results :D

[1] FiXme Note: correct the above lines

CHAPTER

4 CONCLUSION

Conclude.... conclude.... conclude....

BIBLIOGRAPHY

Appendix

A MatLab code for smt....

This is how, we write MatLab code in the report

```
close all
clear all
clc
%I am a comment

filename = 'Results.xlsx';
sheet = 4;
xlRange = 'B3:C12';

[v,T,vT] = xlsread(filename, sheet, xlRange);
x10=v(:,1);y10=v(:,2);

figure
plot(??)
legend(??)

xlim([??])
ylim([??])

title(??)
xlabel('x')
ylabel('y')
```