FYS3150 - Project 2

Dag Arne Lydvo
(Dated: September 27, 2021)

GITHUB REPO:

https://github.com/daglyd/Computational_Physics/tree/main/project_2

PROBLEM 1

With the definition $\hat{x} = \frac{x}{L}$ show that Eq.(4) can be written as Eq.(5). We have equation 4:

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

$$\gamma \frac{d^2u(x)}{dx^2} = \gamma \frac{d^2u(x)}{d\hat{x}^2} \left(\frac{d\hat{x}}{dx}\right)^2 + \gamma \frac{du(x)}{d\hat{x}} \frac{d^2\hat{x}}{dx^2}$$

$$\gamma \frac{d^2u(x)}{d\hat{x}^2} \frac{1}{L^2} + \gamma \frac{du(x)}{d\hat{x}} \cdot 0 = \gamma \frac{d^2u(x)}{dx^2} \frac{1}{L^2}$$

$$\longrightarrow \frac{\gamma}{L^2} \frac{d^2u(x)}{d\hat{x}^2} = -Fu(x)$$

$$\frac{d^2u(x)}{d\hat{x}^2} = -\frac{FK^2}{\gamma} u(x)$$

This gives equation 5:

$$\frac{d^2u(x)}{dx^2} = -\lambda u(x)$$

Where $\lambda = \frac{-FL^2}{\gamma}$

PROBLEM 2

We have that $\vec{v}_i is a set of orthonormal basis vectors, \vec{v}_i^T \cdot \vec{v}_i = \delta_{ij}$.

$$\vec{w}_i^T \cdot \vec{w}_i = (\boldsymbol{U} \cdot \vec{v}_i)^T (\boldsymbol{U} \cdot \vec{v}_i)$$

$$= \boldsymbol{U}^T \cdot \vec{v}_i^T \cdot \boldsymbol{U} \cdot \vec{v}_i$$

$$= \vec{v}_i^T \cdot \boldsymbol{U}^T \boldsymbol{U} \vec{v}_i$$

$$= \vec{v}_i \cdot I \cdot \vec{v}_i$$

$$= \vec{v}_i^T \cdot \vec{v}_i$$

PROBLEM 3

The 6x6 matrix was set up with the tridiagonal signature of $(-1/h^2, 2/h^2, -1/h^2)$. Solving the eigenvalue equation using armadillo's eig_sym produces eigenvalues exactly equal to the analytical solutions. The eigenvectors seems to correspond mostly to the analytical solution, though with some vectors having the sign reversed. I have not been able to figure out the reason for this. See graphic below.

```
6x6 Matrix:
============
   72.0000  -36.0000         0         0         0         0
  -36.0000   72.0000  -36.0000         0         0         0
         0  -36.0000   72.0000  -36.0000         0         0
         0         0  -36.0000   72.0000  -36.0000         0
         0         0         0  -36.0000   72.0000  -36.0000
         0         0         0         0  -36.0000   72.0000

Eigenvalues - Analytical Eigenvalues
====================================
   0.0340   0.0340
   0.1291   0.1291
   0.2667   0.2667
   0.4193   0.4193
   0.5569   0.5569
   0.6520   0.6520

Eigenvectors
============
  -0.2319  -0.4179   0.5211  -0.5211   0.4179  -0.2319
  -0.4179  -0.5211   0.2319   0.2319  -0.5211   0.4179
  -0.5211  -0.2319  -0.4179   0.4179   0.2319  -0.5211
  -0.5211   0.2319  -0.4179  -0.4179   0.2319   0.5211
  -0.4179   0.5211   0.2319  -0.2319  -0.5211  -0.4179
  -0.2319   0.4179   0.5211   0.5211   0.4179   0.2319

Analytical Eigenvectors
=======================
   0.2319   0.4179   0.5211   0.5211   0.4179   0.2319
   0.4179   0.5211   0.2319  -0.2319  -0.5211  -0.4179
   0.5211   0.2319  -0.4179  -0.4179   0.2319   0.5211
   0.5211  -0.2319  -0.4179   0.4179   0.2319  -0.5211
   0.4179  -0.5211   0.2319   0.2319  -0.5211   0.4179
   0.2319  -0.4179   0.5211  -0.5211   0.4179  -0.2319
```

PROBLEM 4

The code for this problem is contained in the functions max_offdiag_symmetric() and problem_4(). The function for finding the max value of the offdiagonal elements seems to be working as it should, the test runs without throwing any errors.

PROBELM 5

When implementing the Jacobi's rotation method the eigenvalues and eigenvectors produces does not match the analytical solution. They seem to be close and some elements closer than others.

```
Problem 5
-----------------
Matrix A (6X6)
-----------------
   72.0000  -36.0000         0         0         0         0
  -36.0000   72.0000  -36.0000         0         0         0
         0  -36.0000   72.0000  -36.0000         0         0
         0         0  -36.0000   72.0000  -36.0000         0
         0         0         0  -36.0000   72.0000  -36.0000
         0         0         0         0  -36.0000   72.0000

Eigenvalues - Analytical Eigenvalues
-----------------------------------
   0.0420   0.0340
   0.1470   0.1291
   0.2745   0.2667
   0.4198   0.4193
   0.5473   0.5569
   0.6523   0.6520

Eigenvectors
------------
   0.1641  -0.5462  -0.6014  -0.6014  -0.5135  -0.5135
   0.2314  -0.3848  -0.4871  -0.4167  -0.4574  -0.5126
   0.3848  -0.2314  -0.2986  -0.1598  -0.1673   0.1673
   0.4592   0.1641  -0.1598   0.2986   0.3338   0.3338
   0.5121   0.4592   0.3359   0.3359   0.3534   0.3534
   0.5462   0.5121   0.4167   0.4871   0.5126   0.4574

Analytical Eigenvectors
-----------------------
   0.2319  -0.5211  -0.4179  -0.5211  -0.5211  -0.5211
   0.2319  -0.4179  -0.4179  -0.4179  -0.5211  -0.4179
   0.4179  -0.2319   0.2319  -0.2319   0.2319  -0.2319
   0.4179   0.2319   0.2319   0.2319   0.2319   0.2319
   0.5211   0.4179   0.5211   0.4179   0.4179   0.4179
   0.5211   0.5211   0.5211   0.5211   0.4179   0.5211
```

Figure 1. Printout from terminal for probelm 5.

PROBLEM 6

The rotations done on the non-zero elements of the matrix will affect the other row and column elements and change the value from zero to non-zero. This will then add to the number of iterations needed to get to a value below tolerance. I assume with a dense matrix the number of iterations will increase as there are more elements far from zero and the behaviour from the sparse example will still exist.

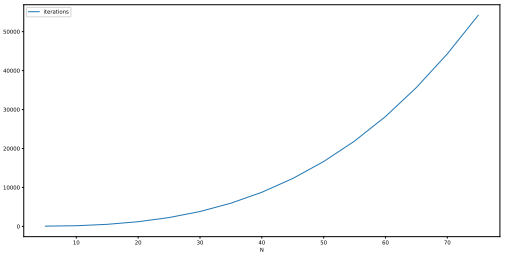

Figure 2. Number of iterations over N.

PROBLEM 7

problem a) n=10 steps.

The eigenvectors calculated using the Jacobi rotation method somewhat seems to resemble the analytical ones. Though the eigenvalues doesn't match, and this is then not surprising. Also two of the plotted eigenvectors seems to be inverted version of the analytical ones.

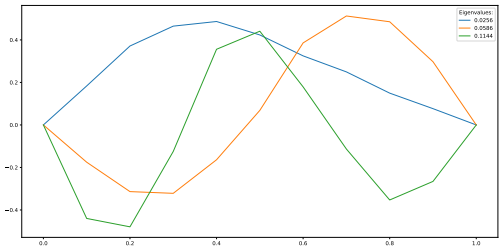

Figure 3. Eigenvectors corresponding to the three smallest eigenvalues from the Jacobi rotation method, using $n = 10$ steps.

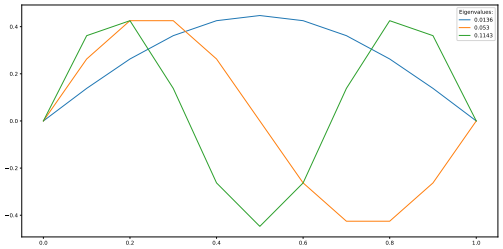

Figure 4. Analytical eigenvectors corresponding to the three smallest eigenvalues, using $n = 10$ steps.

problem b) n=100 steps

Not what I had expected. The calculated eigenvectors using 100 steps does not match the analytical ones. The shapes seems to be very unrealistic, and I suspect there are some error in my algorithm. Yet there could be some overall resemblance in the shapes of the curves corresponding to the analytical ones.

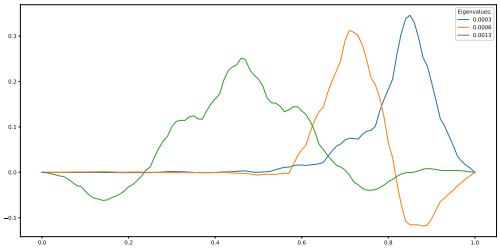

Figure 5. Eigenvectors corresponding to the three smallest eigenvalues from the Jacobi rotation method, using $n = 100$ steps.

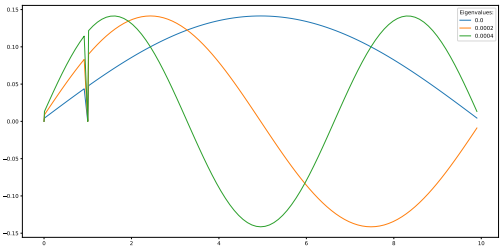

Figure 6. Analytical eigenvectors corresponding to the three smallest eigenvalues, using $n = 100$ steps.s