

Project 2

Sverre Wehn Noremsaune & Frida Marie Engøy Westby
(Dated: September 26, 2021)

<https://github.uio.no/comPhys/FYS3150/tree/project2/project2>

PROBLEM 1 - SECOND ORDER DIFFERENTIAL EQUATION

In this problem we are looking at:

$$\gamma \frac{d^2 u(x)}{dx^2} = -Fu(x) \quad (1)$$

and

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

We know from the assignment that $\hat{x} \equiv x/L \Rightarrow x = \hat{x}L$ and $\lambda = \frac{FL^2}{\gamma}$, and by applying this, we can see that (2) is the scaled version of (1):

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

Put in $x = \hat{x}L$:

$$\begin{aligned} \frac{d^2 u(\hat{x}L)}{d(\hat{x}L)^2} &= -\frac{Fu(\hat{x}L)}{\gamma} \\ \frac{d^2 u(\hat{x})L}{d(\hat{x})^2 L^2} &= -\frac{Fu(\hat{x})L}{\gamma} \end{aligned}$$

Then we multiplies both sides with L :

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

Now we can use $\lambda = \frac{FL^2}{\gamma}$ and we easily see that we get (2). ■

PROBLEM 2 - JACOBI'S ROTATION ALGORITHM

From the assignment we have:

- \vec{v}_i is a set of orthonormal basis vectors: $\vec{v}_i^T \cdot \vec{v}_i = \delta_{ij}$
- \mathbf{U} is an orthogonal transformation matrix: $\mathbf{U}^T = \mathbf{U}^{-1}$

From this we can show that transformations with \mathbf{U} preserves orthonormality, i.e. that $\vec{w}_i = \mathbf{U}\vec{v}_i$ will also be an orthonormal set:

$$\vec{w}_i^T \cdot \vec{w}_j = (\mathbf{U}\vec{v}_i)^T (\mathbf{U}\vec{v}_j) = \vec{v}_i^T \mathbf{U}^T \mathbf{U} \vec{v}_j = \vec{v}_i^T \mathbf{U}^{-1} \mathbf{U} \vec{v}_j = \vec{v}_i^T \mathbf{I} \vec{v}_j = \vec{v}_i^T \cdot \vec{v}_j = \delta_{ij} \quad \blacksquare$$

PROBLEM 3 - THE TRIDIAGONAL MATRIX A

See 'triag.cpp' for code and 'test_triag.cpp' for test.

PROBLEM 4 - LARGEST OFF-DIAGONAL ELEMENT

Problem a

See 'max_offdiag_symmetric.cpp'.

Problem b

See 'test_max_offdiag_symmetric.cpp'.

PROBLEM 5 - IMPLEMENTATION OF JACOBI'S ROTATION

Problem a

See 'jacobi_eigensolver.cpp'.

Problem b

See 'test_jacobi_eigensolver.cpp'.

PROBLEM 6 - TRANSFORMATIONS

Problem a

See 'estimate_rotations.cpp' and FIG 1.

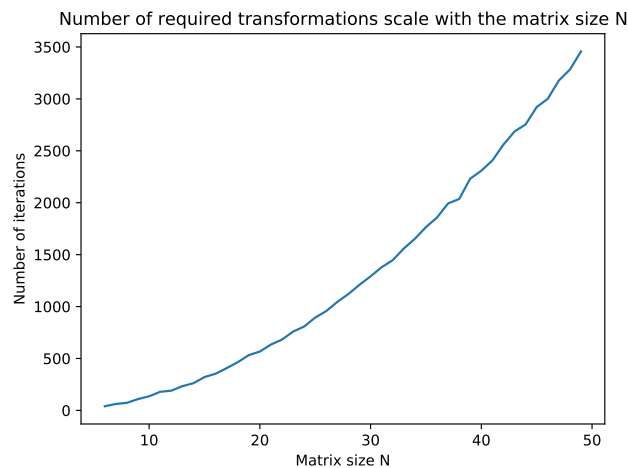


FIG. 1. Number of required transformations scale with the tridiagonal matrix of size N

Problem b

The scaling behavior we expect to see if \mathbf{A} was a dense matrix is that instead of having a $\mathcal{O}(n^2)$ we have $\mathcal{O}(n^3)$.

PROBLEM 7 - EIGENVALUE PROBLEM

Problem a

See 'solve_diff.cpp' and FIG 2.

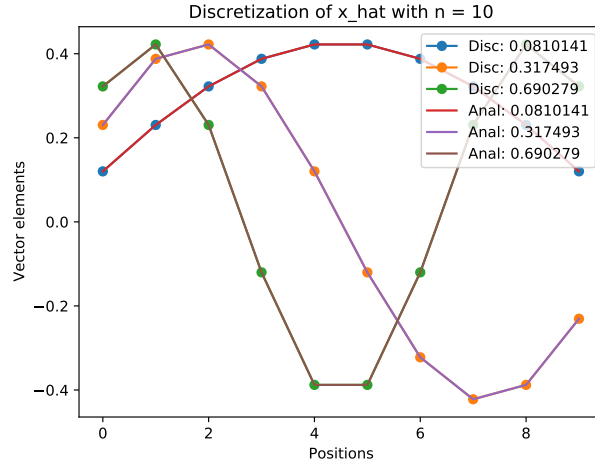


FIG. 2. Plot of the discrete eigenvectors the and corresponding analytical eigenvectors for $N = 10$

Problem b

See 'solve_diff.cpp' and FIG 3.

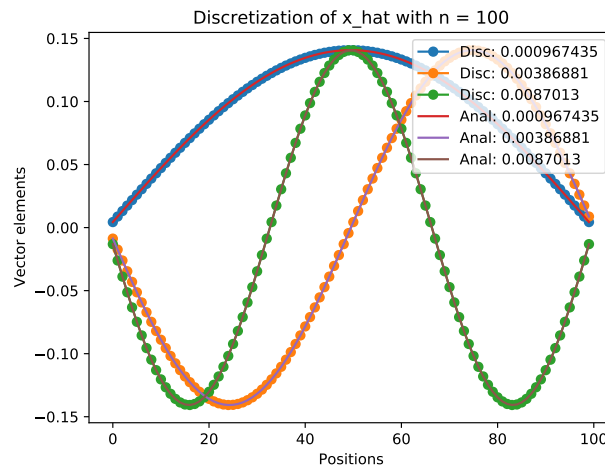


FIG. 3. Plot of the discrete eigenvectors the and corresponding analytical eigenvectors for $N = 100$