FYS3150 - Project 1

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Abstract om du vil

I. THEORY

A. Matrix formulation of the discrete one-dimensional Poisson equation

The one-dimensional Poisson equation with Dirichlet boundary conditions is given by equation 1.

$$-\frac{\mathrm{d}^2 u(x)}{\mathrm{d}x^2} = f(x), \quad x \in (0,1), \quad u(0) = u(1) = 0 \tag{1}$$

We defnine the discretized approximation to u to be v_i at points $x_i = ih$ evenly spaced between $x_0 = 0$ and $x_{n+1} = 1$. The step length between the points is $h = 1/(n+1)$. The boundary conditions from equation 1 then give $v_0 = v_{n+1} = 0$. An approximation to the second derivative of u, derived from the Taylor expansion, is

$$\frac{-v_{i-1} + 2v_i - v_{i+1}}{h^2} = f_i \quad for i = 1, 2, ..., n \tag{2}$$

where $f_i = f(x_i)$.

Written out for all i, equation 2 becomes

$$\begin{aligned}
-v_0 + 2v_1 - v_2 &= h^2 f_1 \\
-v_1 + 2v_2 - v_3 &= h^2 f_2 \\
&... \\
-v_{n-2} + 2v_{n-1} - v_n &= h^2 f_{n-1} \\
-v_{n-1} + 2v_n - v_{n+1} &= h^2 f_n
\end{aligned}$$

In general, this can be rearranged slightly so that

$$\begin{aligned}
2v_1 - v_2 &= h^2 f_1 + v_0 \\
-v_1 + 2v_2 - v_3 &= h^2 f_2 \\
&... \\
-v_{n-2} + 2v_{n-1} - v_n &= h^2 f_{n-1} \\
-v_{n-1} + 2v_n &= h^2 f_n + v_{n+1}
\end{aligned}$$

This system of equations can be written in matrix form as

$$\boldsymbol{Av} = \tilde{\boldsymbol{b}}, \tag{3}$$

explicitly

$$\begin{bmatrix} 2 & -1 & 0 & 0 & ... & 0 \\ -1 & 2 & -1 & 0 & ... & 0 \\ . & & & & & \\ . & & & & & \\ . & & & & & \\ 0 & ... & 0 & -1 & 2 & -1 \\ 0 & ... & 0 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ . \\ . \\ . \\ v_{n-1} \\ v_n \end{bmatrix} = \begin{bmatrix} h^2 f_1 + v_0 \\ h^2 f_2 \\ . \\ . \\ . \\ h^2 f_{n-1} \\ h^2 f_n + v_{n+1} \end{bmatrix}$$

With $v_0 = v_{n+1} = 0$, the right side reduces to $\tilde{b}_i = h^2 f_i$.

B. Solve matrix equation

In order to solve the tridiagonal matrix below we need to develop an algorithm. As mentioned in the exercise set we first need to do a decomposition and forward substitution.

$$\mathbf{Av} = \begin{bmatrix} b_1 & c_1 & 0 & \dots & \dots & \dots \\ a_1 & b_2 & c_2 & \dots & \dots & \dots \\ & a_2 & b_3 & c_3 & \dots & \dots \\ & \dots & \dots & \dots & \dots & \dots \\ & & & a_{n-2} & b_{n-1} & c_{n-1} \\ & & & & a_{n-1} & b_n \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \dots \\ \dots \\ \dots \\ v_n \end{bmatrix} = \begin{bmatrix} \tilde{b}_1 \\ \tilde{b}_2 \\ \dots \\ \dots \\ \dots \\ \tilde{b}_n \end{bmatrix}.$$

Looking at the first matrix multiplication we get the following expression.

$$b_1 v_1 + c_1 v_2 = \tilde{b} \implies v_1 + \alpha_1 v_2 = \rho_1, \quad \alpha_1 = \frac{c_1}{b_1} \wedge \rho_1 = \frac{\tilde{b}_1}{b_1} \tag{4}$$

Doing the second matrix multiplication we get

$$a_1 v_1 + b_2 v_2 + c_2 v_3 = \tilde{b}_2 \tag{5}$$

If we multiply equation 4 by a_1, and subtract it from equation 5 the resulting expression becomes

$$\begin{aligned}
(b_2 - \alpha_1 a_1) v_2 + c_2 v_3 &= \tilde{b}_2 - \rho_1 a_1 \\
\implies v_2 + \frac{c_2}{b_2 - \alpha_1 a_1} v_3 &= \frac{\tilde{b}_2 - \rho_1 a_1}{b_2 - \alpha_1 a_1} \\
\implies v_2 + \alpha_2 v_3 &= \rho_2 \\
\text{where} \quad \alpha_2 = \frac{c_2}{b_2 - \alpha_1 a_1} &\wedge \rho_2 = \frac{\tilde{b}_2 - \rho_1 a_1}{b_2 - \alpha_1 a_1}
\end{aligned}$$

Noticing the pattern in ρ and α we can generalize the terms.

$$\alpha_i = \frac{c_i}{b_i - \alpha_{i-1}a_{i-1}} \quad \text{for} \quad i = 2, 3, ..., n-1 \tag{6}$$

$$\rho_i = \frac{\tilde{b}_i - \rho_{i-1}a_{i-1}}{b_i - \alpha_{i-1}a_{i-1}} \quad \text{for} \quad i = 2, 3, ..., n \tag{7}$$

Inserting the terms into the matrix above, we get a much simpler set of equations.

$$\mathbf{Av} = \begin{bmatrix} 1 & \alpha_1 & 0 & \dots & \dots & \dots \\ 0 & 1 & \alpha_2 & \dots & \dots & \dots \\ & 0 & 1 & \alpha_3 & \dots & \dots \\ & \dots & \dots & \dots & \dots & \dots \\ & & & 0 & 1 & \alpha_{n-1} \\ & & & & 0 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \dots \\ \dots \\ \dots \\ v_n \end{bmatrix} = \begin{bmatrix} \rho_1 \\ \rho_2 \\ \dots \\ \dots \\ \dots \\ \rho_n \end{bmatrix}.$$

Now the last step is to do a backward substitution. Starting with $v_n = \rho_n$ we can work our way backward, with the general expression

$$v_{i-1} = \rho_{i-1} - \alpha_{i-1}v_i \quad \text{for} \quad i = n, n-1, ..., 2 \tag{8}$$

[1] Engeland, Hjorth-Jensen, Viefers, Raklev og Flekkøy, 2020, *Kompendium i FYS2140 Kvantefysikk, Versjon 3*, s. 81
[2] Griffiths, D. J, Schroeter, D. F., 2018, *Introduction to Quantum Mechanics, Third edition*, s. 44

II. APPENDIX

III. KODE