

Project 1 in FYS4150

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Abstract

The aim of this numerical experiment is to solve the one-dimensional Poisson equation with Dirichlet boundary conditions. At first we will use the formula $\mathbf{A}\mathbf{v} = \mathbf{p}$ and the fact that A is a tridiagonal matrix to develop an algorithm that we then can compare to more general methods. We found that: **Write what you found!**

Introduction

Theory

In this project we want to look closer at the one-dimensional Poisson's equation given as:

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Phi}{\partial r} \right) = -4\pi \rho(r) \quad (1)$$

where Φ is the electrostatic potential generated by a localized charge distribution $\rho(r)$. If we now do the substitution $\Phi(r) = \frac{\phi(r)}{r}$, we can rewrite equation (1) as follows:

$$\frac{\partial \phi}{\partial r^2} = -4\pi r \rho(r)$$

By letting $\phi \rightarrow u$ and $r \rightarrow x$ we end up with:

$$-u''(x) = f(x), \quad x \in (0, 1), \quad u(0) = u(1) = 0 \quad (2)$$

If we define the discretized approximation to u as v_i , the second derivative of u can be approximated with:

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

Where $x_i = ih$ are grid points in the interval $x_0 = 0$ to $x_{n+1} = 1$ with step length $h = 1/(n+1)$ and $f_i = f(x_i)$. With the boundary conditions $v_0 = v_{n+1} = 0$ we can see that for $i = 0$ we get:

$$-v_1 + 2v_0 = f_0 h^2$$

For $i = 1$:

$$-v_2 - v_0 + 2v_1 = f_1 h^2$$

For $i = 2$

$$-v_3 - v_1 + 2v_2 = f_2 h^2$$

We can easily see that this gives us:

$$\underbrace{\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & 0 & -1 & 2 \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ \vdots \\ \vdots \\ v_n \end{pmatrix}}_{\mathbf{v}} = \underbrace{\begin{pmatrix} f_1 h^2 \\ f_2 h^2 \\ f_3 h^2 \\ \vdots \\ \vdots \\ \vdots \\ f_n h^2 \end{pmatrix}}_p$$

By setting $f_i h^2 = p_i$ we can write this as:

$$\mathbf{A} \cdot \mathbf{v} = \mathbf{p}$$

The task **Referanse** asks us to make a general algorithm to solve this scenario for any values in the tridiagonal matrix. Assuming a general tridiagonal 4x4-matrix $\tilde{\mathbf{A}}$ for simplicity we can illustrate the method for finding v as follows:

$$\begin{pmatrix} b_1 & c_1 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 \\ 0 & a_3 & b_3 & c_3 \\ 0 & 0 & a_4 & b_4 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{pmatrix}$$

This gives us the following equations:

$$\begin{aligned} \text{I} : v_1 b_1 + c_1 v_2 &= p_1 \\ \text{II} : a_2 v_1 + b_2 v_2 + c_2 v_3 &= p_2 \\ \text{III} : a_3 v_2 + b_3 v_3 + c_3 v_4 &= p_3 \\ \text{IV} : a_4 v_3 + b_4 v_4 &= p_4 \end{aligned}$$

We want only zeroes on the left side of the diagonal:

$$\begin{aligned} p_2^* &= p_2 - p_1 \cdot \frac{a_2}{b_1} \\ &= a_2 v_1 + b_2 v_2 + c_2 v_3 - v_1 a_2 - v_2 \frac{c_1 a_2}{b_1} \\ &= v_2 \left(b_2 - \frac{c_1 a_2}{b_1} \right) + c_2 v_3 \\ &= v_2 b_2^* + c_2 v_3 \end{aligned}$$

Now we have the following matrix:

$$\begin{pmatrix} b_1 & c_1 & 0 & 0 \\ 0 & b_2^* & c_2 & 0 \\ 0 & a_2 & b_3 & c_3 \\ 0 & 0 & a_3 & b_4 \end{pmatrix}$$

As we can see, the a_2 -term disappears from the second row. Following this trail of thought we do the same for the next row.

$$\begin{aligned} p_3^* &= p_3 - p_2 \cdot \frac{a_3}{b_2^*} \\ &= v_3(b_3 - \frac{c_2 a_3}{b_2^*}) + c_3 v_4 \\ &= v_3 b_3^* + c_3 v_4 \end{aligned}$$

This gives us the general idea and we can write a general expression for both p_i^* and b_i^* :

$$p_i^* = p_i - p_{i-1} \frac{a_i}{b_{i-1}^*}, \quad \text{for } i = 2, \dots, n \quad (3)$$

$$b_i^* = b_i - \frac{c_{i-1} a_i}{b_{i-1}^*}, \quad \text{for } i = 2, \dots, n \quad (4)$$

Using equations (4) and (3) through the whole matrix is called forward substitution and we end up with:

$$\begin{pmatrix} b_1 & c_1 & 0 & 0 \\ 0 & b_2^* & c_2 & 0 \\ 0 & 0 & b_3^* & c_3 \\ 0 & 0 & 0 & b_4^* \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2^* \\ p_3^* \\ p_4^* \end{pmatrix}$$

We want to find an expression for v_i and from the last row we can find a simple equation for v_4

$$b_4^* v_4 = p_4^* \Rightarrow v_4 = \frac{p_4^*}{b_4^*}$$

From the second last row we find an expression for v_3

$$b_3^* v_3 + c_3 v_4 = p_3^* \Rightarrow v_3 = \frac{p_3^* - c_3 v_4}{b_3^*}$$

Again, doing this for the next row (going downward and up) we find that v_i can be expressed in a general way as:

$$v_i = \frac{p_i^* - c_i v_{i+1}}{b_i^*}, \quad \text{for } i = 1, \dots, n-1, \quad \text{and } v_n = \frac{p_n^*}{b_n^*} \quad (5)$$

This is called backwards substitution.

Since our v_i is an approximation to the known solution u_i we can find the relative error by:

$$\epsilon_i = \log_{10} \left(\left| \frac{v_i - u_i}{u_i} \right| \right) \quad (6)$$

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Programs

In this section I will present the different key parts of my program.

General tridagional solver

Results

Discussion

Conclusion