FYS4150 - Project 1

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Abstract

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I. Introduction

This project will examine different techniques for approximating the solution to a differential equation where a continious function is known. The equation describes an electrostatic potential Φ generated by a localized charge density $\rho(\vec{r})$ and is usualy described - in three dimentions - by:

$$\nabla^2 \Phi = -4\pi\rho(\vec{r}) \tag{1}$$

If $\rho(\vec{r})$ is spherical symmetric, eq. 1 may be written in a one-dimentional manner by substituting $\phi(r) = r\Phi(r)$:

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

By rewriting eq. 2 to a general form it reads:

$$-u''(x) = f(x) \tag{3}$$

In this spesific case, the Poisson equation is solved by *Gaussian elimination* of a set of linear equations, both in a general manner and an optimized way of a spesific matrix. The optimized method is later compared with another general method called *LU-decomposition*.

*A thank you or further information

II. Methods

The methods used in this projects are the following:

- Dirichlet boundary conditions
- Nummerical derivation
- Gaussian elimination
- LU-decomposition

i. Dirichlet boundary condition

Dirichlet boundary conditions - also refered to as fixed boundary condition - specifies the value of a given function on a surface $T = f(r, t)$. In a one-dimentional problem it translates to defining an interval of x - $x \in [x_{min}, x_{max}]$ - and the function values $f(x_{min}) = f_l$ and $f(x_{max}) = f_h$ at the edges of the intervall.

ii. Nummerical derivarion

The derivative of a discrete funtion may be found by nummerical derivation. The principle of nummerical derivation is a result of Taylor expansion. By expanding a function from a point x with a step h, two equations form depending on the direction:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) \dots \quad (4)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) \dots \quad (5)$$

By adding eq. 5 to eq. 4, a approximation for the second derivative is achieved.

$$f'' = \frac{f_+ - 2f + f_-}{h^2} + \frac{h^4}{6h^2} f^{IV} \quad (6)$$

Where $f_+ = f(x+h)$, $f = f(x)$, $f_- = f(x-h)$ and f^{IV} is the fourth derivative of $f(x)$. By truncating the series at the fourth derivative a small mathematical error - $\mathcal{O}$ - appears in the order of h^2. If a discrete funtion is introduced where $f_i = f(x_i) = f(c_0 + ih)$, eq. 6 may be rewritten to an algorithm for the nummerical second derivative.

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \quad (7)$$

In eq. 7 the mathematical error $\mathcal{O}(h^2)$ is neglected.

iii. Gaussian elimination

Gaussian elimination is a method for simplifying a set of linear equations. It is easly visualized through a matrix notation of $Ax = y$ where A and y is known.

$$\begin{bmatrix} a_0 0 & a_0 1 & a_0 2 \\ a_1 0 & a_1 1 & a_1 2 \\ a_2 0 & a_2 1 & a_2 2 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix} \quad (8)$$

Gaussian elimination is often divided into two main parts, forward and backward substitution.

Forward substitution

The forward substitution is focusing on reducing the number of variables in the set of linear equations to a minimum. In other words, row reduction is used on the matrix A to eliminate all elements a_{i1} where $i < 1$. Turning the matrix equation to $Bx = \hat{y}$:

$$\begin{bmatrix} b_0 0 & b_0 1 & b_0 2 \\ 0 & b_1 1 & b_1 2 \\ 0 & b_2 1 & b_2 2 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \\ \hat{y}_2 \end{bmatrix} \quad (9)$$

where $\hat{y}$ is affected by the row reduction. The process is repeated until matrix A is transformed to an upper triangular matrix A'

$$\begin{bmatrix} a_0 0 & a_0 1 & a_0 2 \\ 0 & a_1 1 & a_1 2 \\ 0 & 0 & a_2 2 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \\ \hat{y}_2 \end{bmatrix} \quad (10)$$

This set of linear equations is the basis for backward substitution.

Backward substitution

The concept of backwars substitution is to solve the the set of equations from bottom to top, and substitute the revealed x_i into the equation above. In the end, all elements of x is known.

iv. LU-decompostition

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