

Project 1: Computational Physics - FYS3150

Fredrik Hoftun & Mikkel Metzsch Jensen

September 09, 2020

Contents

1	Introduction	2
2	Method	2
2.1	Defining the problem	2
2.2	Rewritting the problem as a set of linear equations	3
2.3	General solution using Gaussian elimination	4
2.4	Simplified specific solution	5
2.5	LU decomposition	6
2.6	Comparing precision and error	6
2.7	Implementation	6
3	Results	7
3.1	General algorithm	9
3.2	Special algorithm	9
3.3	LU decomposition	9
4	Discussion	9
5	Conclusion	10
6	References	10

Abstract

The goal of this project were to...
What did we do?
What did we find?

1 Introduction

In this project we will investigate different numerical approaches for the solving of the one-dimensional Poisson equation with Dirichlet boundary conditions. This is a problem that is used in many different scientific applications. It is used to describe electrostatic and magnetostatic phenomena in a quantitative manner. It also helps to understand diffusion and propagation problems. The solution is generally used in a wide range of fields such as engineering, physics, mathematics, biology, chemistry, etc. [1]. In this project we have used a second derivative approximation in order to rewrite the problem as a set of linear equations. We have written three different algorithms: A general and a specialized algorithm using gaussian elimination and then LU decomposition. These are described individually in the method sections along with a calculation of the number of floating point operations for each of them. Since we know the analytical solution for our problem we have compared relative error for different choices of stepsize h in the algorithm. We have also compared the CPU time of these computations. We found a significant difference in both precision (due to round off errors) and CPU time, which are presented in the results section.

1. Motivate the reader
2. What have I done
3. The structure of the report
4. conclusion?

2 Method

2.1 Defining the problem

We are going to solve the one-dimensional Poisson equation with Dirichlet boundary conditions given as the following:

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

In our case we will use the function:

$$f(x) = 100e^{-10x}$$

Note that the algorithms for solving the problem will not be dependent on this specific choice of $f(x)$. The reason why we stick to this function is for the practicality of having the following analytical solution for $f(x)$:

$$u(x) = 1 - (1 - e^{-10})x - e^{-10x}$$

We can ensure that this is a valid solution by inserting it into the Poisson equation. First we calculate double derivative of $u(x)$:

$$u'(x) = -(1 - e^{-10}) + 10e^{-10x}, \quad u''(x) = -100e^{-10x}$$

We now see that the solution satisfies the Poisson equation:

$$-u''(x) = 100e^{-10x} = f(x)$$

We can therefore use this analytical solution to evaluate the precision of the numerical solutions for different choices of step length h .

2.2 Rewriting the problem as a set of linear equations

In order to solve the Poisson equation numerically we discretize u as v_i with $n + 2$ grid points $x_i = ih$ for $i = 0, 1, \dots, n + 1$. To clarify we have $x_0 = 0, x_{n+1} = 1$ which are spaced with step length $h = 1/(n + 1)$. The boundary conditions is then $v_0 = v_{n+1} = 0$. We use the following second derivative approximation

$$-u''(x_i) \approx -\frac{v_{i+1} + 2v_i - v_{i-1}}{h^2} = f(x_i) \quad \text{for } i = 1, \dots, n$$

\Leftrightarrow

$$-v_{i-1} + 2v_i - v_{i+1} = h^2 f(x_i)$$

Notice that we cannot calculate the second derivative approximation at the end points $i = 0$ and $i = n + 1$ since we need available points $v_{\pm 1}$ for the calculation. We define the column vector $\mathbf{v} = [v_1, v_2, \dots, v_n]$ and try to setup the equation for every step $i = 1, \dots, n$. As we do this we see a useful pattern appearing

$$\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} = h^2 f(x_1)$$

$$\begin{bmatrix} 2 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & \cdots \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} = h^2 \begin{bmatrix} f(x_1) \\ f(x_2) \end{bmatrix}$$

\vdots

$$\begin{bmatrix} 2 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & \cdots \\ 0 & -1 & 2 & -1 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & & -1 & 2 & -1 \\ 0 & \cdots & & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} = h^2 \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f_n \end{bmatrix}$$

From this we see that we can write the problem as a linear set of equation:

$$\mathbf{A}\mathbf{v} = \mathbf{g}$$

With the following definitions:

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & \cdots \\ 0 & -1 & 2 & -1 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & & -1 & 2 & -1 \\ 0 & \cdots & & 0 & -1 & 2 \end{bmatrix}, \mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}, \tilde{\mathbf{g}} = h^2 \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f_n \end{bmatrix}$$

2.3 General solution using Gaussian elimination

We can solve our set of linear equations generally using Gaussian elimination on the matrix $\mathbf{A}\mathbf{v} = \mathbf{g}$, where we now define a more generalized matrix (A) as:

$$A = \begin{bmatrix} b_1 & c_1 & 0 & \cdots & \cdots & 0 \\ a_1 & b_2 & c_2 & 0 & \cdots & \cdots \\ 0 & a_2 & b_3 & c_3 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & & a_{n-2} & b_{n-1} & c_{n-1} \\ 0 & \cdots & & 0 & a_{n-1} & b_n \end{bmatrix}$$

where a_i are the elements below the diagonal, b_i are the elements on the diagonal and c_i are the elements above the diagonal. This gives us the algorithm: We can calculate the algorithm's number of Floating Point Opera-

Algorithm 1 General algorithm

```

1: for  $i = 2, \dots, n$  do                                 $\triangleright$  Forward substitution eliminating  $a_i$ 
2:    $b_i = b_i - c_{i-1} \cdot a_i / b_{i-1}$                        $\triangleright$  Update  $b_i$ 
3:    $g_i = g_i - g_{i-1} \cdot a_i / b_{i-1}$                    $\triangleright$  Update  $g_i$ 
4: end for

5:  $v_n = g_n / B_n$ ;                                          $\triangleright$  Backward substitution obtaining  $v_i$ 
6: for  $i = n - 1, \dots, 1$  do
7:    $v_i = \frac{g_i - c_i \cdot v_{i+1}}{b_i}$ 
8: end for
  
```

tions. Each arithmetic operation is one FLO(PS). So in our forward substitution we have $2 \cdot 3$ FLOPS and in the backward substitution we have $1 + 3$ FLOPS. The forward substitution goes from 2 to n , totaling $n - 2$ points. The backward substitution also has $n - 2$ points. Then the total number of FLOPS are:

$$(6 + 3)(n - 2) + 1 = 9n - 17$$

2.4 Simplified specific solution

In this specific case we have $a = -1$, $b = 2$, $c = -1$ which means we can further simplify our matrix \mathbf{A} :

$$\begin{aligned}
 \mathbf{A} &= \begin{bmatrix} 2 & -1 & 0 & \dots & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & \dots \\ 0 & -1 & 2 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & & -1 & 2 & -1 \\ 0 & \dots & & 0 & -1 & 2 \end{bmatrix} \sim \begin{bmatrix} 2 & -1 & 0 & \dots & \dots & 0 \\ 0 & 3/2 & -1 & 0 & \dots & \dots \\ 0 & -1 & 2 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & & -1 & 2 & -1 \\ 0 & \dots & & 0 & -1 & 2 \end{bmatrix} \\
 &\sim \begin{bmatrix} 2 & -1 & 0 & \dots & \dots & 0 \\ 0 & 3/2 & -1 & 0 & \dots & \dots \\ 0 & 0 & 4/3 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & & -1 & 2 & -1 \\ 0 & \dots & & 0 & -1 & 2 \end{bmatrix} \sim \begin{bmatrix} 2 & -1 & 0 & \dots & \dots & 0 \\ 0 & 3/2 & -1 & 0 & \dots & \dots \\ 0 & 0 & 4/3 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & & 0 & i_n/i_n - 1 & -1 \\ 0 & \dots & & 0 & 0 & i_n + 1/i_n \end{bmatrix}
 \end{aligned}$$

Where we have called the last diagonal element i_n . We see that $b_i = \frac{i+1}{i}$, reducing the computation time. With our new b_i we can create a new algorithm.

Algorithm 2 Special algorithm, where $a_i = -1$, $b_i = 2$, $c_i = -1$

```

1: for  $i = 2, \dots, n$  do                                ▷ Forward substitution eliminating  $a_i$ 
2:    $b_i = i + 1/i$                                          ▷ Update  $b_i$ 
3:    $g_i = g_i + g_{i-1}/b_{i-1}$                                ▷ Update  $g_i$ 
4: end for

5:  $v_n = 0$                                                 ▷ Backward substitution obtaining  $v_i$ 
6: for  $i = n - 1, \dots, 1$  do
7:    $v_i = \frac{g_i + v_{i+1}}{b_i}$ 
8: end for

```

Similarly to the general algorithm we can calculate total FLOPS:

$$(2 * 2 + 2)(n - 2) + 1 = 6n - 11$$

Which for large n is considerably less. If we take into account that $b_i = \frac{i+1}{i}$ can be precalculated for all $i \in [1, \dots, n]$ before hand, we get a total number of FP:

$$(2 + 2)(n - 2) = 4n - 8$$

which for large n can be approximated to $4n$

2.5 LU decomposition

For the LU decomposition we ...

FLOPS $O(n^3)$ se https://en.wikipedia.org/wiki/LU_decomposition, søk etter "float"

2.6 Comparing precision and error

2.7 Implementation

We used C++ to implement our algorithms ... and we used Python's library Matplotlib to plot our results.

3 Results

GITHUB LINK HERE

Max error:

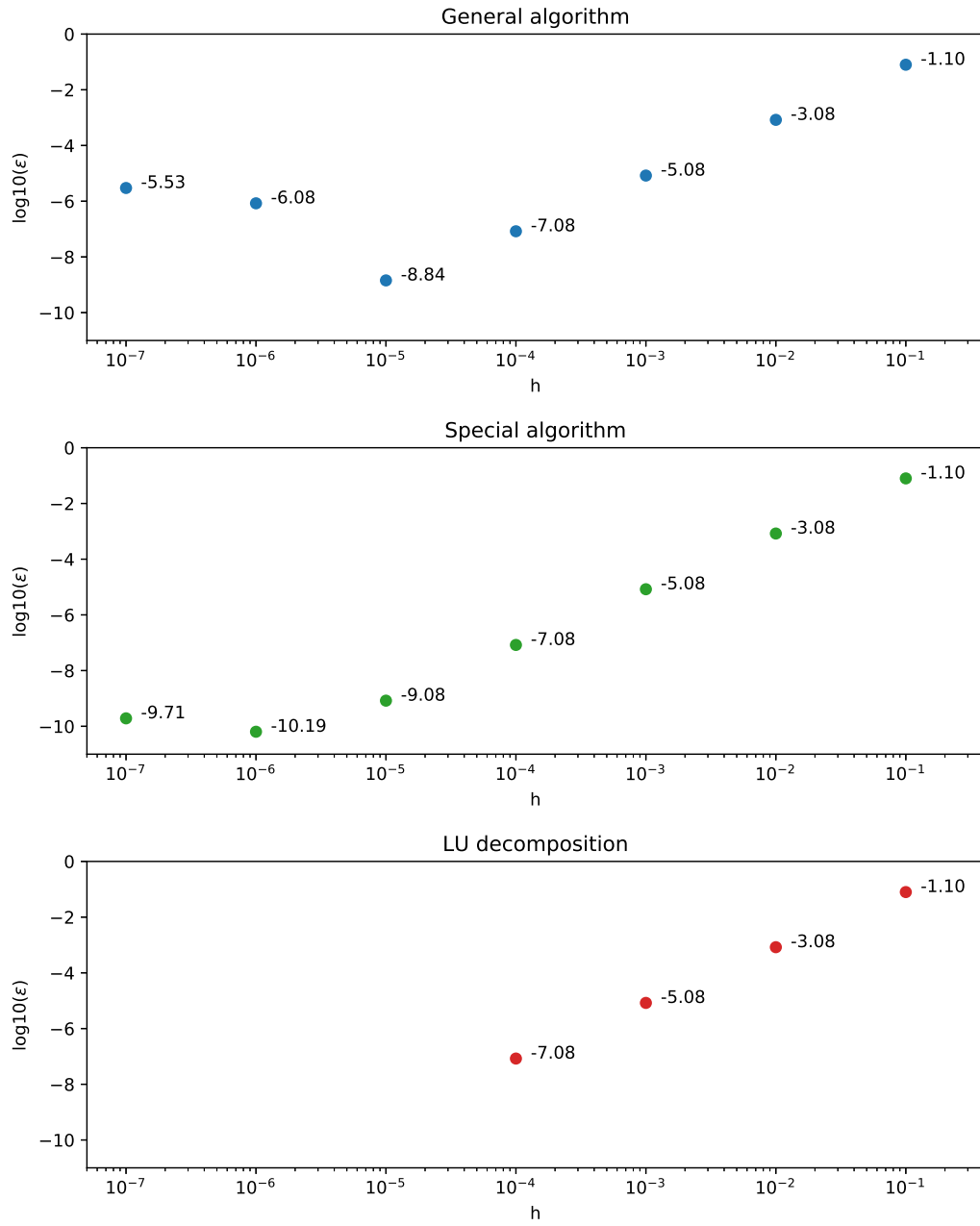


Figure 1: Log10 of the maximum error for each numerical solution compared to the analytical solution for different number of gridpoints n and different numerical methods.

Table 1: CPU Time

N	General algorithm [s]	Special algorithm	LU Decomposition
10^1	3×10^{-6}	3×10^{-6}	9.81×10^{-4}
10^2	4×10^{-6}	4×10^{-6}	1.96×10^{-4}
10^3	3.8×10^{-5}	3.7×10^{-5}	1.02×10^{-2}
10^4	3.41×10^{-4}	3.54×10^{-4}	2.45
10^5	3.79×10^{-3}	3.50×10^{-3}	nan
10^6	3.57×10^{-2}	3.24×10^{-2}	nan
10^7	3.16×10^{-1}	3.24×10^{-1}	nan

Computer specs:

CPU = 2.5 GHz Intel Core i5

3.1 General algorithm

3.2 Special algorithm

3.3 LU decomposition

4 Discussion

Error analysis

The computer should be able to make a maximum of $2.5e9$ floating point operations pr. second. We can investigate the number of FLOPS for the general algorithm with $n = 10^7$:

$$FP = 9 \times 10^7 - 17 \approx 9 \times 10^7$$

$$\text{CPU Time} = 0.316 \text{ s}$$

$$\text{FLOPS} = FP / \text{CPU Time} \approx 0.28 \text{ GHz}$$

We see that there is some room up the maximum capacity of the processor (2.5 GHz), but this might be somewhat expectable

5 Conclusion

In this report we have used three different ways of computing $\mathbf{Av} = \mathbf{g}$ and have seen that efficiency of the methods vary greatly. We have witnessed the importance of efficient implementation of algorithms ...

6 References

References

- [1] S. B. Gueye, K. Talla and C. Mbow, "Solution of 1d poisson equation with neumann-dirichlet and dirichlet-neumann boundary conditions using the finite difference method", Journal of Electromagnetic Analysis and Applications, Vol. 6, No. 10, pp. 309, 2014.