Project 1

FYS4150 - Computational Physics

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1 Introduction

The purpose of this project is to develop an algorithm that will be used to find a numerical solution to the one-dimensional Poisson equation

$$-u''(x) = f(x), \tag{1}$$

where $x \in (0,1)$, with the Dirichlet boundary conditions $u(0) = u(1) = 0$. It will be assumed that the source term ($f(x)$) takes the form

$$f(x) = 100e^{-10x}. \tag{2}$$

The solution we obtain numerically will be compared to a closed-form solution given by

$$u(x) = 1 - \left(1 - e^{-10}\right) x - e^{-10x}. \tag{3}$$

We can easily show that this is a solution to eq. (1) by taking the first and second derivatives:

$$\begin{aligned} & u'(x) = -\left(1 - e^{-10}\right) + 10e^{-10x} \\ \Rightarrow \quad & u''(x) = -100e^{-10x} \\ \Rightarrow \quad & -u''(x) = 100e^{-10x} = f(x). \end{aligned}$$

The algorithm will be developed in two different stages; first a general one, and then a simplified one that deals with the particular problem in this project. The two versions of the algorithm will be compared in terms of number of floating point operations and CPU time.

Another important part of the project is to study the error of the numerical solution, and how it evolves as we decrease the step size in the algorithm. Finally we will also solve the equation by using library functions, and see why this might not be a good idea.

2 Discretization of the Poisson equation

To solve something numerically we need to make a discrete approximation to the problem. In this case we approximate $u(x)$ by $v(x_i) = v_i$, with $x_i = ih$ in the interval $x_0 = 0$ to $x_{n+1} = 1$. The step size is defined by $h = 1/(n+1)$. The boundary conditions are now given by $v_0 = v_{n+1} = 0$.

The second derivative is approximated by

$$u''(x) \approx \frac{v_{i+1} + v_{i-1} - 2v_i}{h^2}, \tag{4}$$

meaning that our problem can be written as

$$-\frac{v_{i+1} + v_{i-1} - 2v_i}{h^2} = f_i, \tag{5}$$

where $f_i = f(x_i)$ and $i = 1, \ldots, n$. To simplify the expression a little bit we multiply both sides by h^2, and define $y_i = h^2 f_i$.[1]

Let us now write eq. (5) explicitly for some values of i (and keep in mind that $v_0 = v_{n+1} = 0$):

$$\begin{aligned} i = 1 \quad &\Rightarrow \quad -v_2 + 2v_1 = y_1 \\ i = 2 \quad &\Rightarrow \quad -v_3 - v_1 + 2v_2 = y_2 \\ i = 2 \quad &\Rightarrow \quad -v_4 - v_2 + 2v_3 = y_3 \\ &\vdots \\ i = n \quad &\Rightarrow \quad -v_{n-1} + 2v_n = y_n \end{aligned}$$

It is now relatively easy to see that this can be written as a matrix equation if we define

$$\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \quad \text{and} \quad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}.$$

The equation can then be written as $\mathbf{Av} = \mathbf{y}$, where $\mathbf{A}$ is the tridiagonal $n \times n$-matrix given by

$$\mathbf{A} = \begin{pmatrix} 2 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & \cdots \\ 0 & -1 & 2 & -1 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & \cdots & 0 & -1 & 2 \end{pmatrix},$$

meaning that to solve the problem we need to solve this equation for $\mathbf{v}$.

3 Developing the algorithm

When solving a matrix equation we make use of Gaussian elimination. A general tridiagonal matrix can be written in terms of vectors a, b and c as

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

[1] In the project description it is suggested to use $\tilde{b}_i = h^2 f_i$, but I found that this can be quite confusing, as b is used to denote the diagonal elements of the matrix $\mathbf{A}$, meaning that $\tilde{b}$ is very convenient to use when doing the Gauss elimination.

so what we actually want to do is to eliminate all a's in the matrix. We see that to eliminate a_1 we must multiply the first row by $\frac{a_1}{b_1}$, and then subtract it from the second row, meaning that the second row becomes

$$\begin{pmatrix} 0 & b_2 - \frac{c_1 a_1}{b_1} & c_2 & 0 & \cdots & 0 \end{pmatrix}.$$

(Notice that the c's are not affected by this procedure.) To simplify the expressions we would like to define

$$\tilde{b}_2 \equiv b_2 - \frac{c_1 a_1}{b_1}.$$

The procedure then continues in the same pattern, and we realize that the new diagonal elements ($\tilde{b}$'s) can be written as

$$\tilde{b}_i = b_i - \frac{a_i c_{i-1}}{\tilde{b}_{i-1}}. \tag{6}$$

We must also remember to do the same operations on the right hand side,

$$\tilde{f}_i = y_i - \frac{a_i \tilde{f}_{i-1}}{\tilde{b}_{i-1}}. \tag{7}$$

The procedure of updating $\tilde{b}_i$ and $\tilde{f}_i$ is referred to as *forward substitution*.

When the elimination is done we need to do a *backwards substitution* to actually solve the equation for each v_i. Since we now have a diagonal matrix we should start at the last equation, i.e. $\tilde{b}_n v_n = \tilde{f}_n$, which means that

$$v_n = \frac{\tilde{f}_n}{\tilde{b}_n}.$$

Now that v_n is known we can move to the second last equation, solve it for v_{n-1}, and so on. The general expression for v_i becomes

$$v_i = \frac{\tilde{f}_{i+1} - c_i v_{i+1}}{\tilde{b}_i}.$$

Before moving on to how I have coded this, and finally look at results, I would like to get all the "maths" done by looking at how we in our case can simplify the above expressions.

3.1 Simplifying the algorithm

We have now looked at how the matrix equation is solved when **A** is a general tridiagonal matrix. However, the matrix we are studying is simplified quite a bit, as all $a_i = c_i = -1$, while all $b_i = 2$. The first thing to notice is that eq. (6) can be written as

$$\tilde{b}_i = 2 - \frac{1}{\tilde{b}_{i-1}}.$$

By writing the first few terms

$$\tilde{b}_2 = 2 - \frac{1}{2} = \frac{3}{2}, \quad \tilde{b}_3 = 2 - \frac{1}{3/2} = \frac{4}{3}, \quad \tilde{b}_4 = 2 - \frac{1}{4/3} = \frac{5}{4},$$

and so on, we realize that we can actually write the $\tilde{b}$'s as

$$\tilde{b}_i = \frac{i+1}{i}.$$

By doing the same for the $\tilde{f}$'s we find that

$$\tilde{f}_i = y_i + \frac{i-1}{i}\tilde{f}_{i-1} = y_i + \frac{\tilde{f}_i}{\tilde{b}_{i-1}},$$

and finally

$$v_{i-1} = \frac{i-1}{i}(\tilde{f}_{i-1} - v_i) = \frac{\tilde{f}_{i-1} - v_i}{\tilde{b}_{i-1}}.$$

When doing these simplifications the total number of floating point operations (FLOPS) is reduced quite a bit. Since $\tilde{b}_i$ only depends on i the full $\tilde{\mathbf{b}}$ can be calculated before starting the algorithm, which reduces the number of FLOPS from $6(n-1)$ to $2(n-1)$ in the forward substitution, and from $3n$ to $2n$ in the backwards substitution.

3.2 Coding the algorithm

At the moment of writing this report I have only written the code in Python, and the code can be found in the following git-repository:

https://github.com/evensha/FYS4150/tree/master/Project1

The program take two input arguments:

1. An argument that specify if we want to run the general or the simplified algorithm ("g" for general and "s" for simplified).

2. The matrix dimension, n.

When writing the code I have chosen to let all arrays have $n + 2$ elements, i.e. $i = 0, 1, \ldots, n, n + 1$, to make the arrays correspond to the total number of grid points (including the boundary points), and to make the code as close to the mathematical expressions as possible.

After making the necessary arrays (a, b, c, x, f and v) I make the four different loops, i.e. forward and backward substitution in both the general and the simplified way. The loops just update the values of the array elements of b, f and v, meaning that I have chosen not to make separate arrays called $\tilde{b}$, $\tilde{f}$, and so on. While running the algorithm I also calculate the CPU time. When the algorithm is done I make an

array for the closed form solution, and plot it together with the numerical solution from the algorithm, and the (logarithm of) the relative error is calculated by the formula

$$\epsilon_i = log_{10}\left(\left|\frac{v_i - u_i}{u_i}\right|\right). \tag{8}$$

All results are shown in the next section.

The last part of the program is to solve the problem by using library functions. I have chosen to use functions from the `scipy` library, which for instance contains the `lu()`-function for LU decomposition, and `inv()` for inverting a matrix. The CPU time is calculated for this procedure as well.

4 Results

Figure 1 shows the numerical solution plotted together with the closed-form solution for 10, 100 and 1000 grid points. When $n = 10$ we can see that the numerical estimate is somewhat different from the analytical solution, while for $n = 100$ and $n = 1000$ they seem to be very similar. (If one zooms closely in on the $n = 100$ plot it is possible to see a slight difference around the maximum of the curve, while for $n = 1000$ there seems to be no observable difference between the curves.)

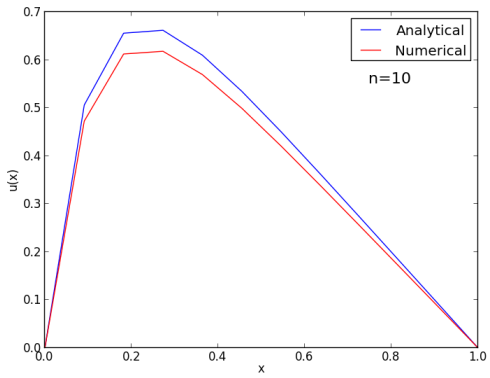
The point of developing the simplified algorithm is of course to reduce the amount of time we spend on solving the problem. The CPU time for spent for the two different algorithms are given in Table 1. We see that for $n = 10$ the CPU time is almost the same, while for larger values of n the simplified algorithm is about twice as fast as the general one.

	CPU time (s)	
n	General alg.	Simplified alg.
10^1	$3.5 \cdot 10^{-5}$	$3.1 \cdot 10^{-5}$
10^2	$3.3 \cdot 10^{-4}$	$1.8 \cdot 10^{-4}$
10^3	$3.3 \cdot 10^{-3}$	$1.7 \cdot 10^{-3}$
10^4	$3.2 \cdot 10^{-2}$	$1.7 \cdot 10^{-2}$
10^5	0.33	0.17
10^6	3.28	1.66

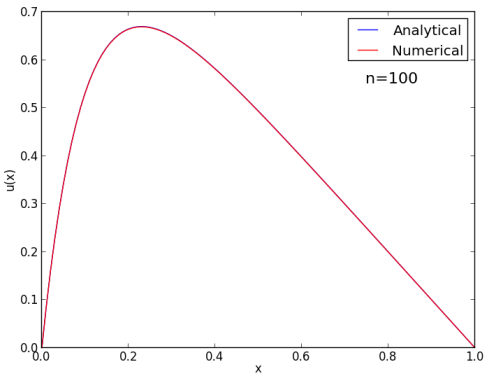
Table 1: CPU time comparisons for the two algorithms.

In Table 2 the *log-log* relation between h and ϵ_i (defined in eq. (8)) is given. By considering the mathematical truncation error we expect that ϵ_i increases by a factor of 2 when n is increased by a factor of 10. We see in the table that this holds up to and including $n = 10^4$. After this the error seems to be more "random", which must be due to limited numerical precision.

5 Conclusions



(a)



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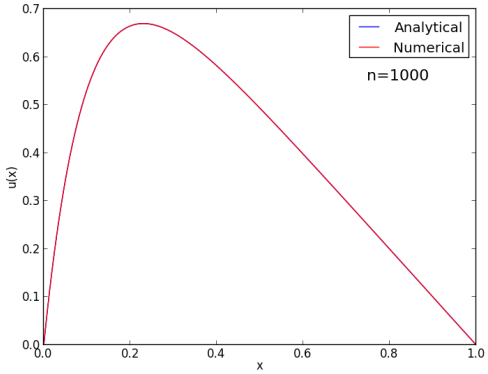

(c)

Figure 1: Analytical and numerical solutions for $n = 10$, 100 and 1000.

n	$log_{10}(h)$	ϵ_i
10^1	-1.041	-1.180
10^2	-2.004	-3.088
10^3	-3.000	-5.080
10^4	-4.000	-7.079
10^5	-5.000	-8.843
10^6	-6.000	-6.075
10^7	-7.000	-5.525

Table 2: ϵ_i as function of $log_{10}(h)$.