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 $\mathbf{Av} = \mathbf{p}$ and the fact that A is a tridiagnoal matrix to devlope a specialized algorithm that we then can compare to more general methods. We found that a specialized algorithm is better than a general and that using LU-decomposition is the slowest method. The relative error of the approximation compared to the exact solution is best at $\log_{10}(h) = -5$ where h is the step length.

Introduction

This projects goal is to teach the students that giving a computer less things to do but still doing the same thing, makes it do the things you want it to do faster. [3] To do this we are going to sovle the one-dimensional Poisson's equation with different numerical methods. We are going to focus on three main methods. The first method will be a general method which also can be used to solve similar cases in the future. Building upon an approximation of the second derivative of $u(x)$ we create a tridiagonal matrix and by using forward and backward substitution we will solve $\mathbf{Av} = \mathbf{p}$ where $\mathbf{A}$ is our matrix and $\mathbf{p}$ is known.
When we have found a general method we will use the fact that in this case we have a tridiagonal matrix with one value along each diagonal to optimze our code for this special case. Thirdly, we will use the more robust LU-decomposition.

Afterwards we will measure the time each method uses and find the relative error of our aproximation. Doing all this will gives us a better knowledge of the usage of vectors and matrices in C++ and dynamic memory allocation.

The project was done in cooperation with Simen Nyhus Bastnes, but because of a sick family member I had to go away and could not deliver on time with him. Because we use the same program and have worked together our reports may be similar, but we have written one each.

Theory

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

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

where Φ is the electrostatic potential generated bya localized charge distribution $\rho(r)$. If we 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 $\phi \to u$ and $r \to x$ we end up with:

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

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

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

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:

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

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

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

The task asks us to make a general algorithm to solve this scenario for any values in the tridiagonal matrix. Assuming a general tridiagonal 4x4-matrix $\widetilde{\mathbf{A}}$ 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:

$$\begin{aligned} \text{I} &: v_1 b_1 + c_1 v_2 &&= p_1 \\ \text{II} &: a_2 v_1 + b_2 v_2 + c_2 v_3 &&= p_2 \\ \text{III} &: a_3 v_2 + b_3 v_3 + c_3 v_4 &&= p_3 \\ \text{IV} &: a_4 v_3 + b_4 v_4 &&= p4 \end{aligned}$$

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

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

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 disappers from the second row. Following this trail of thought we do the same for the next row.

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

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

$$p_i^* = p_i - p_{i-1} \frac{a_i}{b_{i-1}^*}, \quad \text{for i = 2,...,n,} \quad \text{and } p_1^* = p_1 \tag{3}$$

$$b_i^* = b_i - \frac{c_{i-1} a_i}{b_{i-1}^*}, \quad \text{for i = 2,...,n,} \quad \text{and } b_1^* = b_1 \tag{4}$$

Using equations (4) and (3) through the whole matrix is called forward substitution and our expression becomes:

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

We also need 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 to 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 downwards and up) we find that v_i can be expressend in a general way as:

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

This is called backwards substitution.

However, since **A** has the same values for a, b and c for all i, we can specialize equations (3), (4) and (5). By inserting $a_i = c_i = -1$ and $b_i = 2$ in (4) we can easily see that:

$$b_i^* = \frac{i+1}{i}, \quad \text{for i = 2,...,n,} \quad \text{and } b_1^* = b_1 = 2 \tag{6}$$

$$p_i^* = p_i + \frac{p_{i-1}^*}{b_{i-1}^*}, \quad \text{for i = 2,...,n,} \quad \text{and } p_1^* = p_1 \tag{7}$$

$$v_i = \frac{p_i^* + v_{i+1}}{b_i^*}, \quad \text{for i = n-1,...,1,} \quad \text{and } v_n = \frac{p_n^*}{b_n^*} \tag{8}$$

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

$$\epsilon_i = \log_{10}\left(\left|\frac{v_i - u_i}{u_i}\right|\right) \tag{9}$$

where the known solution u_i is given as:

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

LU-decompostion

Another method that can be used is the method of LU-decompostion. If the determinant of a matrix **A** is different from zero, we can factorize **A** into a lower diagonal matrix **L** and an upper diagonal matrix **U**:

$$\mathbf{A} = \mathbf{LU}$$

$$\begin{pmatrix} a_{1,1} & \cdots & \cdots & a_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ a_{n,1} & \cdots & \cdots & a_{n,n} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ l_{2,1} & \ddots & & \vdots \\ \vdots & & \ddots & 0 \\ l_{n,1} & \cdots & l_{n,n-1} & 1 \end{pmatrix} \begin{pmatrix} u_{1,1} & u_{1,2} & \cdots & u_{1,n} \\ 0 & u_{2,2} & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & 0 & u_{n,n} \end{pmatrix}$$

Using this in our original expression gives us:

$$\mathbf{LUv} = \mathbf{p}$$

Rewriting this we get:

$$\mathbf{Ly} = \mathbf{p}, \quad \mathbf{Uv} = \mathbf{y}$$

This is solvable by using backwards substitution to find $\mathbf{y}$ and then use that to find $\mathbf{v}$. Usually, for LU-decomposition and backwards substitution, solving it goes as $\mathcal{O}(\frac{2}{3}n^3)$. For more information about the method, see the wikipedia [2]

Programs

In this section I will present the different key parts of my program. For the full program, please visit my github. [1]

General tridagional solver

Implementing the equations for forward substitution, (3) and (4), were done as follows:

Algorithm 1 Forward substitution

1: $b_1^* = b_1$
2: $p_1^* = p_1$
3: **for** $i = 2, n$ **do**
4: $\quad b_i^* = b_i - a_{i-1} \cdot c_{i-1}/b_{i-1}^*$
5: $\quad p_i^* = p_i - p_{i-1}^* \cdot a_i/b_{i-1}^*$
6: **end for**

The backward substitution given in equation (5) was written as:

Algorithm 2 Backward substitution

1: $v_n = p_n^*/b_n^*$
2: **for** $i = n-1, 1$ **do**
3: $\quad v_i = (p_i^* - c_i \cdot v_{i+1})/b_i^*$
4: **end for**

Counting number of floating point operations gives us 6 for forward substitution and 3 for backward. This gives us $9n$ FLOPS in total.

Specialized tridagional solver

Since all a and c-values are -1 and all b-values are 2 throughout $\mathbf{A}$, we don't need the general algorithm, but can use a more specialized algorithm. Our specialized algorithm is based on equation (7) and (8) (equation (6) was calculated beforehand) and was implemented as follows:

Algorithm 3 Specialized algorithm

1: $p_1^* = p_1$
2: **for** $i = 2, n$ **do** ▷ Forward substitution
3: $\quad p_i^* = p_i + p_{i-1}^*/d_{i-1}$
4: **end for**
5: $v_n = p_n^*/d_n$
6: **for** $i = n-1, 1$ **do** ▷ Backwards substitution
7: $\quad v_i = (p_i^* + v_{i+1})/d_i$
8: **end for**

This method gives us $4n$ FLOPS.

Results

To see if our approximation with forward and backward substitution was right, we plotted it against the known solution given in equation (10). For a starter we set the n-value to 10, this gave us 10 different x-values. The result where we compare the known and approximated solution is shown in figure 1.

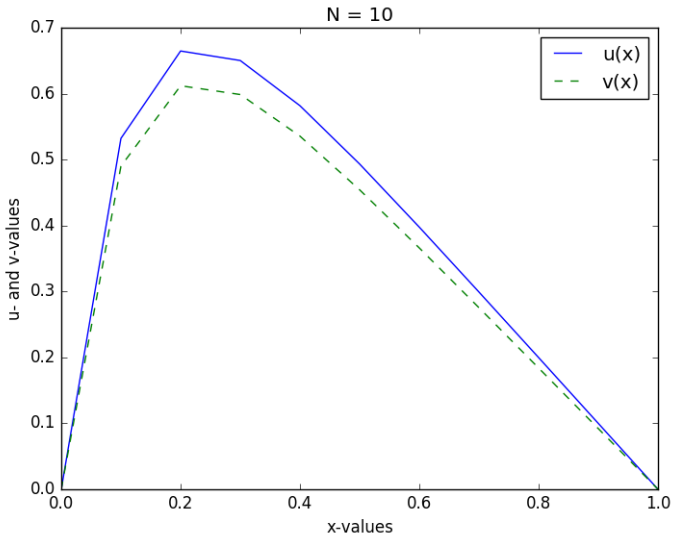
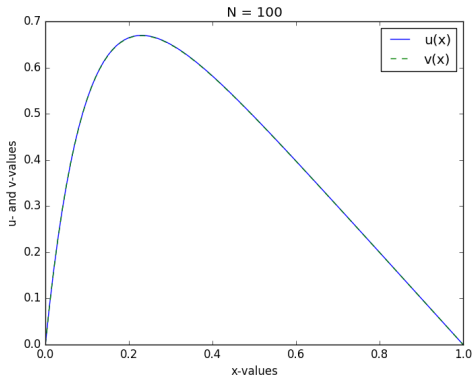
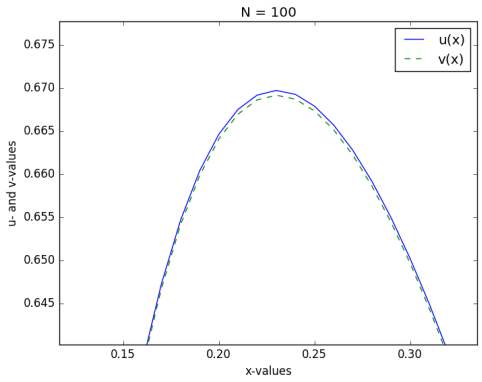


Figure 1: Our first plot where we have n = 10 points. u(x) is the correct solution and v(x) is the approximated. As we can see that they almost align, but not quite. Especially in the top around x = 0.2.

Afterwards we set the n-value to 100 and got 100 points. The result of this can be seen in figure 2. As we can see from figures 2a and 2b we have to zoom in to see any difference. We also ploted for higher values of N, but the results were much the same as for n = 100 only we had to zoom in even more to see the difference.



(a) The n = 100 case



(b) The n = 100 case, zoomed in.

Figure 2: The plot for n = 100. u(x) and v(x) are the same as above. As we can see the graphs are much more aligned now. On the left we have zoomed in on the top to show the small differences.

To see the effectiveness of our specialized algorithm we took the time of the general,the specialized algorithm and the LU-decomposition method. The result is presented in table 1.

$\log_{10}(n)$	General [sec]	Specialized [sec]	LU-decomposition [sec]
1	$2.0 \cdot 10^{-6}$	$1.0 \cdot 10^{-6}$	$8.0 \cdot 10^{-6}$
2	$4.0 \cdot 10^{-6}$	$2.0 \cdot 10^{-6}$	$4.3 \cdot 10^{-3}$
3	$5.3 \cdot 10^{-5}$	$2.7 \cdot 10^{-5}$	2.2
4	$6.0 \cdot 10^{-4}$	$4.2 \cdot 10^{-4}$	-
5	$3.8 \cdot 10^{-3}$	$2.2 \cdot 10^{-3}$	-
6	$4.2 \cdot 10^{-2}$	$2.4 \cdot 10^{-2}$	-
7	0.43	0.26	-

Table 1: This table shows us the time used by the program for different n-values. The last column contains only 3 values because for n = 10000 and above the calculations took too long.

Lastly we found the relative error using equation (9) and the result is presented in table 2.

$log_{10}(h)$	Relative error
-1	-1.1
-2	-3.1
-3	-5.1
-4	-7.1
-5	-9.0
-6	-6.8
-7	-13.5

Table 2: The relative error between our approximation and the exact solution as a function of step length h.

Discussion

Comparing our three methods we can see that the specialized algorithm is superior when it comes to time usage. From table 1 we can see that there is about a factor of two between the general and the specialized algorithm. This fits almost with our estimation of respectivevly $9n$ and $4n$ FLOPS. We can also see that the LU-decomposition is clearly inferior. This is becuase the technique calculates with a whole matrix, while our method with forward and backward substitution only uses values in the three diagonals. In our case with such small n-values one can debate if it really was necessary to make a specialized algorithm when the general method only used 0.43 seconds with $n = 10^7$. It is a fair point, however, if we had continued with higher values of n until the program used about half an hour completing the task, I would prefere the method that only used 15 minutes. And with larger values of n we meet another problem. If we continued to high enough values of n, we would have overflow and then the program would not work even if it only used half the time to do it.
If I had done this assignment again in the future, I would want to look over my program with fresh eyes and try to make it more effective. I would have liked to find a more efficient way to do the LU-decomposition. Even if it it is not the most effective in the tridiagonal case, it is always useful to have a good way to manipulate whole matrices at once.

From figures 1 and 2 we can clearly see that for these small values, increasing n will give a better approximation. This is also confirmed by table 2 which shows us that the relative error decreases until we reach $\log_{10}(h) = -5$. After that it becomes larger and then it becomes smaller again. Why we have this sudden peak at $\log_{10}(h) = -6$ is unclear to me. It may be round of errors or it may be that this exact number of steps gives an uncertainty not present elsewhere. If we increase the step length even further we can see that for $\log_{10}(h) = -8$, we have a relative error at about -2, going higher than that makes my computer crash. This could mean two things: Either we have an anomaly at $\log_{10}(h) = -6$ and the relative error here should be lower or we have an anomaly at $\log_{10}(h) = -8$ and the relative error here should be higher. It would be natural to assume that $\log_{10}(h) = -5$ is the optimal and that afterwards the relative error becomes worse and worse. If I were to do the project again, I would look more into this and run the program for smaller step lengths on a computer with more RAM.

Conclusion

At the end of the day it is clear that the specialized algorithm uses the shortest time and is thus the optimal way to solve this specific task. The approximation becomes better and better until we reach step lengths as small as $\log_{10}(h) = -5$. Even though $\log_{10}(h) = -8$ gives a better relative error, this could be because of something wrong in the program and should be double checked before it is trusted. The LU-decompostion is a slow method because it uses the whole matrix and does not take advantage of the properties of a tridiagonal matrix.

A little comment

This is aside from the rest of the report, but is a message from me to you who are reading this. When I took experimental physics I learned a lot about writing reports, but I learned it a bit too late. I almost got a grade higher in that course than the one I ended up with. But because of one badly written report (the first one that counted on the grade in that course), I was given a worse grade. One of the teachers said that maybe if he had been stricter with me from the start I would have known what I learned from that one bad report earlier and would have recieved a better grade. Therefore I hope you will be strict with me from the start. I can take it. I would rather feel dumb because of all the mistakes I did in this report than in the reports that count on the final grade.

References

[1] Eirik's github. `https://github.com/scuper42/FYS4150/tree/master/project1`.

[2] Lu-decomposition. `https://en.wikipedia.org/wiki/LU_decomposition`.

[3] Morten Hjorth-Jensen. Project 1. `https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Projects/2016/Project1/project1_2016.pdf`, 2016.