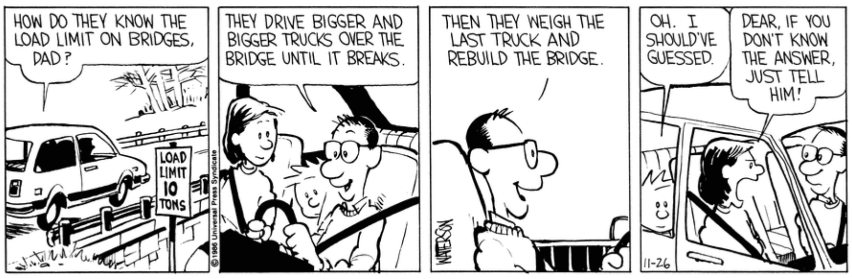
SOLVING THE POISSON-EQUATION IN ONE DIMENSION.

FYS3150

IVAR STANGEBY
GITHUB.COM/QTIPTIP/FYS3150

ABSTRACT. In this project we examine and solve the Poisson equation in one dimension. We consider various numerical methods for solving the discretized differential equation and compare their numerical efficiency.


HOW DO THEY KNOW THE LOAD LIMIT ON BRIDGES, DAD?
LOAD LIMIT 10 TONS
THEY DRIVE BIGGER AND BIGGER TRUCKS OVER THE BRIDGE UNTIL IT BREAKS.
THEN THEY WEIGH THE LAST TRUCK AND REBUILD THE BRIDGE.
OH. I SHOULD'VE GUESSED.
DEAR, IF YOU DON'T KNOW THE ANSWER, JUST TELL HIM!
WATTERSON
11-26

CONTENTS

1. Introduction

In this project we are tasked with solving the one-dimensional Poisson equation. One can look at the project as consisting of three parts. Analytical examination of the problem, numerical solution to the problem, and lastly, comparing our numerical results to our expectations in the first part.

We start by deriving the three point approximation to the second derivative of a function f. We then use this approximation to show that we can rewrite the set of equations as a matrix equation. Our task at hand is then to solve this matrix equation using some algorithm, which in this case is going to be the tridiagonal matrix algorithm (TDMA). We will analyze this algorithm to figure out what kind of results we can expect and we will compare this with the standard Gaussian elimination and LU decomposition methods.

We then implement our devised algorithm and solve our system for various grid-resolutions and compare our results with the closed form solution of our given problem. We will do this visually by plotting the analytical solution against the numerical solution.

Lastly, we want to examine the relative error that occurs for various step sizes and extract the largest relative error over the grid for different resolutions. The motivation behind this is to figure out which resolution (step size) gives the most optimal results. We then compare this to the expectations from part 1.

2. Formulating the problem

2.1. Physical background.

The poisson-equation in three dimensions read

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

where ∇^2 is the Laplacian-operator. In three dimensions it is expressed using spherical coordinates. In this project however, we are going to assume that Φ and ρ are spherically symmetric which essentially mean that the whole equation reduces to a one-dimensional problem in the radius r. Writing out the laplacian for a spherically symmetric system we get

$$\nabla^2 = \frac{1}{r^2}\frac{d}{d2}\left(r^2\frac{d}{dr}\right).$$

If we substitute $\Phi(r) = \phi(r)/r$ our poisson-equation then reads

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

The motivation behind this substitution is to ensure that we achieve the Dirichlet boundary conditions we want.

We finally let $\phi \to u$ and $r \to x$, and the equation now reads

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

The function f is called the *source term*, and in this project we are going to assume that $f(x) = 100e^{-10x}$. We can then compare our results with the closed form solution $u(x) = 1-(1-e^{-10})x - e^{-10x}$. Equation (1) naturally gives rise to the need of a numerical approximation to the second derivative of a function u.

2.2. Approximating the second derivative.

Writing out the Taylor-expansion of a function $f : \mathbb{R} \to \mathbb{R}$ we get

$$f(x) = \sum_{i=0}^{\infty}\frac{f^{(n)}(a)}{n!}(x-a)^n.$$

If we examine that partial sums T_n of this series we are truncating the exact expansion at some n. Note that $f(x) = \lim_{n\to\infty} T_n$.

$$T_n(x) = \sum_{i=0}^{n} \frac{f^{(n)}(a)}{n!}(x-a)^n.$$

By doing this, we are essentially approximating our function f at a point x, and we are introducing a truncation error. We evaluate T_n around $x = a$ at the point $x \pm h$ and achieve

$$T_n(x \pm h) = \sum_{i=0}^{n} \frac{f^{(n)}(x)}{n!} h^n.$$

Setting $n = 2$ we obtain a term containing the second derivative of f,

$$T_2(x \pm h) = f(x) \pm f'(x)h + \frac{f''(x)}{2}h^2,$$

and we now write out the sum of $T_2(x+h)$ and $T_2(x-h)$. This yields

$$\begin{aligned} f(x+h) + f(x-h) &= T_2(x+h) + T_2(x-h) + \mathcal{O}(h^4) \\ &= 2f(x) + f''(x)h^2 + \mathcal{O}(h^4) \end{aligned}$$

which when solved for $f''(x)$ is equal to

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2). \tag{2}$$

This equation is the one we will employ during the solution of the linear system. Note that $\mathcal{O}(h^2)$ is just shorthand for the truncation error introduced by setting $n = 2$. It is an error-function that runs like h^2, however we will take the approximation, so ignoring this error-term. We will later compare the results for various values of h.

2.3. **System of linear equations.**

We want to solve eq. (1) over a discrete set of n distinct points $\{x_i\}_{i=1}^n$ where $x_i = ih$ over the interval $[0, 1]$. We define the step length $h = 1/(n+1)$ and it then follows that $x_0 = 0$ and $x_{n+1} = 1$.

If we now write out eq. (1) using our approximation to the second derivative, namely eq. (2), and denote the discretized approximation to u at a point x_i as v_i then we achieve the following for the discrete point x_i:

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

where $f(x)$ is the source term. Note that we write $f(x_i) = f_i$. In preparation for the next step we multiply through by h^2.

$$-v_{i+1} + 2v_i - v_{i-1} = h^2 f_i \text{ for all } i = 1, \dots, n, \tag{3}$$

We now observe that Equation (3) along with the set of i's define a set of n linear equations. Writing them out, we notice a pattern:

$$\begin{aligned} -v_2 + 2v_1 - v_0 &= h^2 f_1 \\ -v_3 + 2v_2 - v_1 &= h^2 f_2 \\ &\vdots \\ -v_n + 2v_{n-1} - v_{n-2} &= h^2 f_{n-1} \\ -v_{n+1} + 2v_n - v_{n-1} &= h^2 f_n \end{aligned}$$

Remember that we only have n equations and $n+2$ unknowns, hence the Dirichlet boundary conditions are key if we are to solve this system.

This system can be rewritten in terms of a coefficient matrix A, a vector $\mathbf{v}$ consisting of the variables v_i, and a vector $\tilde{\mathbf{b}}$ that consists of $b_i = h^2 f_i$. Our system is now reduced to a matrix equation

$$A\mathbf{v} = \tilde{\mathbf{b}}. \tag{4}$$

Note that A is an $n \times n$ matrix, which does not cover the end cases. Also note that A is a tridiagonal matrix, because only the middle three diagonals are non-zero.

3. Solving the problem

In this section we examine the implementation specific details of this project. We are now going to outline the algorithm known as the *Thomas Algorithm*, or *Tridiagonal Matrix Algorithm.*[1] The Tridiagonal Matrix Algorithm is a special case of LU-decomposition tailored to tridiagonal systems. Due to problems with getting the armadillo *solve()* method to work, I will also implement the standard Gaussian algorithm for comparison.

3.1. **Devising an algorithm.**

In order to solve this matrix equation involving a tridiagonal matrix there are several shortcuts we can take. First note that the matrix is sparse, i.e., that the number of non-zero elements scale as $\mathcal{O}(n)$. In our case, since the elements are all along the three main diagonals we can make significant cuts in the memory by only storing the three diagonals as vectors. This way we only have to store $3n$ of the elements, assuming we only work with vectors of length n.

If we let $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ denote the three main diagonals with elements a_i, b_i, c_i for $i = 1, \ldots, n$ respectively then eq. (3) can be written as

$$a_i v_{i+1} + b_i v + c v_{i-1} = h^2 f_i = \tilde{b}_i.$$

Our goal now is to use the first equation to eliminate v_1 from the second equation, then use the new modified second equation to eliminate v_2 from the third equation and so on. After doing this for all n equations, the final equation is an equation in one variable, namely v_n, which can be used to solve the previous $n-1$ equations. This is an algorithm in two steps, a forward sweep where we forward substitute, and then a backward sweep where we substitute back in to solve the equations. This algorithm scales linearly in the number of grid points. We require $2n$ substitutions, so the algorithm runs in $\mathcal{O}(n)$.

We now wish to decompose A into two triangular matrices. We denote these by L and U respectively. We can now write eq. (4) in terms of these new matrices:

$$LU\mathbf{v} = \tilde{\mathbf{b}}, \tag{5}$$

with

$$A = \begin{bmatrix} \lambda_1 & \ldots & \ldots & \ldots & \ldots & \ldots \\ a_1 & \lambda_2 & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & a_{n-1} & \lambda_{n-1} & \ldots \\ \ldots & \ldots & \ldots & \ldots & a_n & \lambda_n \end{bmatrix} \cdot \begin{bmatrix} 1 & \gamma_1 & \ldots & \ldots & \ldots & \ldots \\ \ldots & 1 & \gamma_2 & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & 1 & \gamma_{n-1} \\ \ldots & \ldots & \ldots & \ldots & \ldots & 1 \end{bmatrix}$$

We start by first solving $L\mathbf{y} = \tilde{\mathbf{b}}$. This gives us the equations

$$y_i = \begin{cases} \frac{\tilde{b}_i}{\lambda_i}, & i = 1 \\ \frac{\tilde{b}_i - a_i y_{i-1}}{\lambda_i}, & i = 2, \ldots, n. \end{cases}$$

And solving $U\mathbf{v} = \mathbf{y}$ yields:

$$v_i = \begin{cases} y_i - \gamma_i v_{i+1}, & i = 1, \ldots, n-1 \\ y_i, & i = n. \end{cases}$$

All we need now is an expression for λ_i and γ_i for $i = 1, \ldots, n$. This follows directly from the fact that $A = LU$.

$$\lambda_i = \begin{cases} b_i, & i = 1 \\ b_i - a_i\gamma_{i-1}, & i = 2, \ldots, n. \end{cases}$$

$$\gamma_i = \frac{c_i}{\lambda_i}, \quad i = 1, \ldots, n.$$

We now have everything we need for solving eq. (5).

The algorithm we will implement is given by fig. 1. It is interesting to note that when implementing this, we can use the same vector for $\mathbf{v}$ and $\mathbf{y}$ as they do not interfere. This saves us some memory.

FIGURE 1. Tridiagonal matrix algorithm

```
comment: Forward sweep
$\lambda_1 = b_1$
$\gamma_1 = \frac{c_1}{\lambda_1}$
$y_1 = \frac{b_1}{\lambda_1}$
for $i = 2, \ldots, n$ do
    $\lambda_i = b_i - a_i\gamma_{i-1}$
    $\gamma_i = \frac{c_i}{\lambda_i}$
    $y_i = \frac{b_i - a_i y_{i-1}}{\lambda_i}$
od
comment: Backward sweep
$v_n = y_n$
for $i = n - 1, \ldots 1$ do
    $v_i = y_i - \gamma_i v_{i+1}$
od
```

We are now interested in the number of floating point operations (FLOPS) this algorithm constitutes. For the forward sweep, there are 2 FLOPS for the initialization, and then 6 for each iteration in the for loop for a total of $6(n-1) + 2$ FLOPS. For the backward sweep, we have $2(n-1)$ FLOPS. For the whole algorithm this is then $8n - 6$ FLOPS. For large n the -6 is negligible and we say that the algorithm spends $8n$ FLOPS. This again verifies the complexity of the algorithm as $\mathcal{O}(n)$.

If we compare this to the standard Gaussian method which require $2n^3/3$ FLOPS [3], which constitutes a complexity of $\mathcal{O}(n^3)$, our algorithm runs a whole lot faster for large n.

3.2. **General solution to LU-decomposed matrix.** Using armadillo's LU-decomposition we achieve an upper and lower triangular matrix. We again wish to solve the equations

$$L\mathbf{y} = \tilde{\mathbf{b}} \text{ and } U\mathbf{v} = \mathbf{y}. \tag{6}$$

The reason we wish to use armadillo's LU-decomposition is we want a more general solution algorithm to our equation in order to compare the run time. Using the same procedure as in the previous section we achieve the more general algorithm outlined in fig. 2.

Figure 2. Gaussian elimination

```
comment: Forward sweep
for $i = 1, \dots, n$ do
    $y_i = \tilde{b}_i$
    for $j = 1, \dots, i-1$ do
        $y_i = y_i - L_{i,j} y_j$
    od
od
comment: Backward sweep
for $i = n, \dots, 1$ do
    $v_i = y_i$
    for $j = i+1, \dots n$ do
        $v_i = v_i - U_{i,j} v_j$
    od
    $v_i = \frac{v_i}{U_{i,i}}$
od
```

3.3. **Algorithm performance.** Logging the average run-time for the various values of n gives us an estimate of how the two methods compare, our *Tridiagonal Matrix Algorithm* and the more general *forward-backward substitution.* The results are given in table 1.

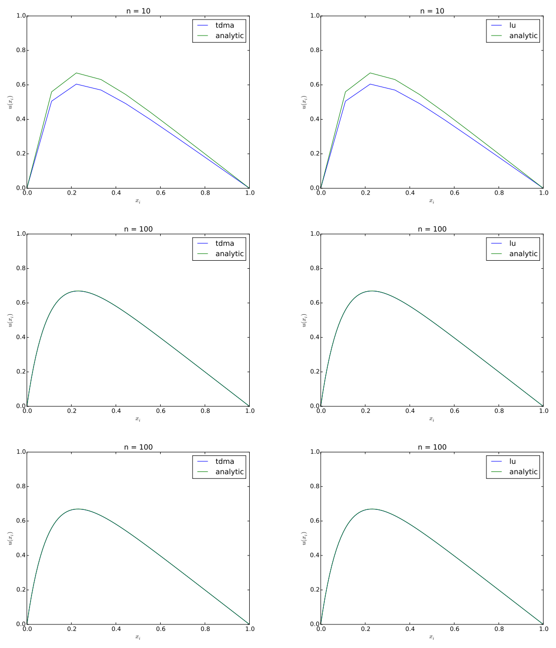
Table 1. Elapsed time for various n

n	tdma[s]	lu[s]
10	0.000003	0.000993
100	0.000009	0.001350
1000	0.000065	0.090025
10000	0.000571	20.386738
100000	0.006204	N/A
1000000	0.058982	N/A

We see that the time required for the LU-decomposition is quite significant compared to the Tridiagonal Matrix Algorithm. It is interesting then to see the differences in the numerical approximation. The results are given in figure 3. As we can see, the numerical approximation is "exact" for $n = 100$, so it converges very quickly. For our case, the LU-method and the Tridiagonal Matrix Algorithm are identical, hence the only difference in performance is the computation needed to decompose A into lower and upper triangular matrices. Therefore, for all intents and purposes, our algorithm is strictly better than the LU-decomposition.

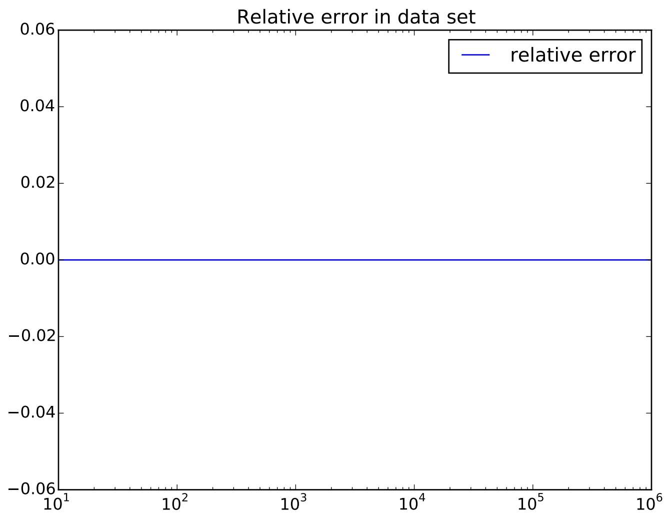
I could not get Armadillo's `solve()` method to work. The results would probably have differed a bit more had the solution to the LU-decomposed method not been implemented by hand.

Figure 3. Numerical approximation for various n



Of interest is also the relative error in our data set using the TDMA for various n. This has been computed and is presented in fig. 5.

Figure 5. Relative error in dataset



The maximum relative error for each time-step is given in table 2. We see that at $n = 10^5$ the error start increasing again due to the error in numerical precision becomes large as h becomes small, as we can see in eq. (2).

TABLE 2. Maximum relative error in data set for various n

n	ε_{max}
10	0.000000
100	0.000000
1000	0.000000
10000	0.000000
100000	0.000000
1000000	0.000000

4. CONCLUSION

Our implementation of the *Tridiagonal Matrix Algorithm* improves vastly on the standard *Gaussian elimination method* and *LU-decomposition* if speed is to be considered. However, our algorithm is just an optimization of the latter methods for use with tridiagonal matrix problems. The main difference between our TDMA and the LU-method we used for comparison is that our TDMA is tailored to this specific problem, while the LU-decomposition method in Armadillo is for a general case. Hence the latter method is much much slower. Other than that, the results are similar and no loss in numerical precision occurs using the one over the other.

In addition, our TDMA is memorypreserving in the sense that it does not have to store each element of a sparse matrix, but just the diagonal vectors. We could even improve on this further, by observing that our diagonal vectors are constant.

4.1. Things to consider.

During this project I learned the importance of planning my implementation of a numerical algorithm before starting to implement it. Knowing how to count, from 1 to n is key. I struggled a bit with layout out the algorithm for the boundary conditions as well as knowing what vector length to use. Having the algorithms written down before starting to implement, as in Figure 1 and 2 helped a lot and I'll keep this in mind for the next projects.

I also spent significant time debugging my `Python`-implementation when the error was in the writing to file in my C++-program.

REFERENCES

[1] *https://en.wikipedia.org/wiki/Tridiagonal_matrix_algorithm*

[2] *http://www.gocomics.com/calvinandhobbes/1986/11/26*

[3] *https://en.wikipedia.org/wiki/Gaussian_elimination#Computational_efficiency*

[4] *Computational Physics - Lecture Notes Fall 2015 - Morten Hjorth-Jensen*