

FYS3150 - project 1

Sverre Wehn Noremsaune & Frida Marie Engøy Westby
(Dated: September 13, 2021)

<https://github.uio.no/comPhys/FYS3150/tree/project1>

PROBLEM 1

We have the one-dimensional Poisson equation

$$-\frac{d^2u}{dx^2} = f(x) \quad (1)$$

where $f(x)$ is known to be $100e^{-10x}$. We also assume $x \in [0, 1]$, that the boundary condition are $u(0) = 0 = u(1)$ and $u(x)$ is

$$u(x) = 1 - (1 - e^{-10})x - e^{-10x} \quad (2)$$

where $u(x)$ is an exact solution to Eq. (1). We can check this analytically by differentiating $u(x)$ twice.

$$\begin{aligned} -u''(x) &= f(x) \\ u''(x) &= -f(x) \\ u(x)' &= 10x^{-10x} - 1 + \frac{1}{e} \\ u''(x) &= -100e^{-10x} = -f(x) \quad \blacksquare \end{aligned}$$

PROBLEM 2

See FIG 1. wich shows the plot of the exact Poisson solution. See 'poisson_exact.cpp' and 'algorithms.cpp' in the github repository, for source code.

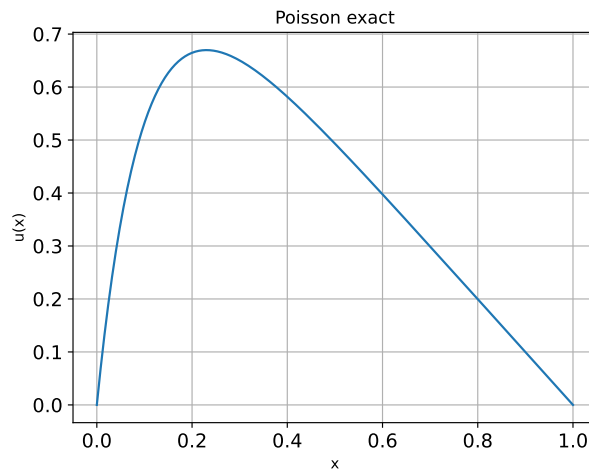


FIG. 1. A plot of the exact solution for the Poisson equation from 1 for $x \in [0, 1]$

PROBLEM 3

We are discretizing the Poisson equation from 1.
Discretizing x and setting up some notation:

$$\begin{aligned} x &\rightarrow x_i \\ u(x) &\rightarrow u_i \\ i &= 0, 1, \dots, n \\ h &= \frac{x_{max} - x_{min}}{n} \\ x_i &= x_0 + ih \end{aligned}$$

Next we're using the three-point formula to find the second derivative:

$$\frac{du^2}{dx^2} = u'' = \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} + O(h^2)$$

$$f_i = - \left(\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} + O(h^2) \right)$$

Then we approximate and change the notation, $v_i \approx u_i$ and get

$$f_i = \frac{-v_{i-1} + 2v_i - v_{i+1}}{h^2} \quad (3)$$

PROBLEM 4

The equation we got in 3 isn't the most ergonomic for setting up a matrix equation, so we can rewrite it to

$$-v_{i-1} + 2v_i - v_{i+1} = h^2 f_i \quad (4)$$

Equation 4 is a set of equations for every i

$$\begin{aligned} i=1 & \quad -v_0 \quad 2v_1 \quad -v_2 &= h^2 f_1 \\ i=2 & \quad \quad -v_1 \quad 2v_2 \quad -v_3 &= h^2 f_2 \end{aligned}$$

and so on and so forth. We can see that v_0 and v_n will end up and alone on their columns, and since we know what they are we simply move them over.

$$\begin{aligned} i=1 & \quad 2v_1 \quad -v_2 &= h^2 f_1 + v_0 \\ i=2 & \quad -v_1 \quad 2v_2 \quad -v_3 &= h^2 f_2 \end{aligned}$$

This can then be easily rewritten as a matrix equation $A\vec{v} = \vec{g}$

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 2 & -1 & 0 \\ 0 & 0 & \dots & 0 & -1 & 2 & -1 \\ 0 & 0 & \dots & 0 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{n-3} \\ v_{n-2} \\ v_{n-1} \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ \vdots \\ gn-3 \\ gn-2 \\ gn-1 \end{bmatrix}$$

where g_i is $h^2 f_i$ ($+v_0$ for f_1 and $+v_n$ for f_{n-1}).

PROBLEM 5**Problem a**

We can see that n is related to m since we're "dropping" 2 columns, which gives $n = m - 2$

Problem b

We will find \vec{v}_i^* for $1..(n - 1)$, meaning everything but the boundary points.

problem 6

Here will we look at a general tridiagonal matrix, and not the Poisson equation from earlier.

Problem a

Algorithm 1 Algorithm for solving general tridiagonal matrix

arrays a , b , c , u , f , $temp$ of length n

$btemp = b[1]$

$u[1] = f[1]/btemp$

for $i = 2, 3, \dots, n$ **do**

$temp[i] = c[i-1] / btemp$

$btemp = b[i] - a[i] * temp[i]$

$u[i] = (f[i] - a[i] * u[i-1]) / btemp$

for $i = n-1, n-2, \dots, 1$ **do**

$u[i] -= temp[i+1] * u[i+1]$

Problem b

When we analyse the algorithm above, we can see that we get $1 + 6(n - 1) + 2(n - 1) = 1 + 8(n - 1) = 8n - 7$ FLOPs.

PROBLEM 7

In this problem and the problems below, will we once again look at the Poisson Equation.

Problem a

See 'general_tridiag.cpp' and 'algorithms.cpp' in the github repository for the program that solves the Poisson equation with the general algorithm.

Problem b

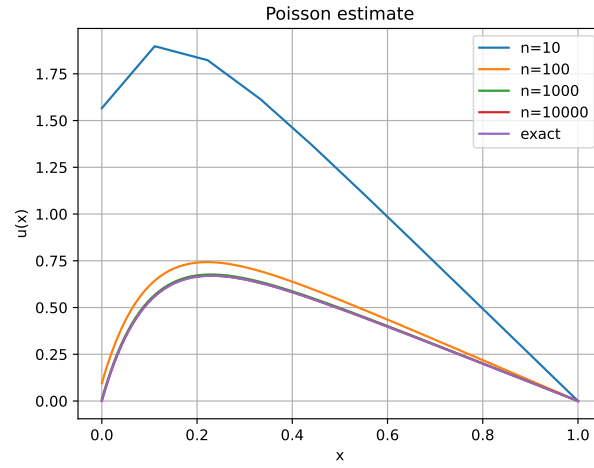


FIG. 2. Exact vs numerical comparison for the solution of equation 1

PROBLEM 8

Problem a

See FIG 3 for the plot showing the (logarithm of) the absolute error.

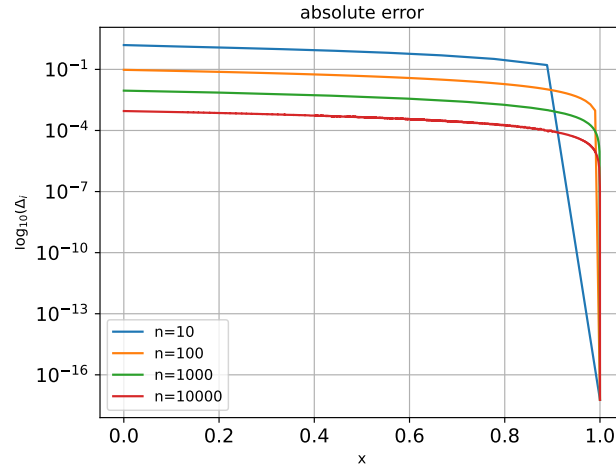


FIG. 3. The absolute error for the general tridiagonal algorithm in \log_{10}

Problem b

See FIG 4 for the plot showing the (logarithm of) the relative error.

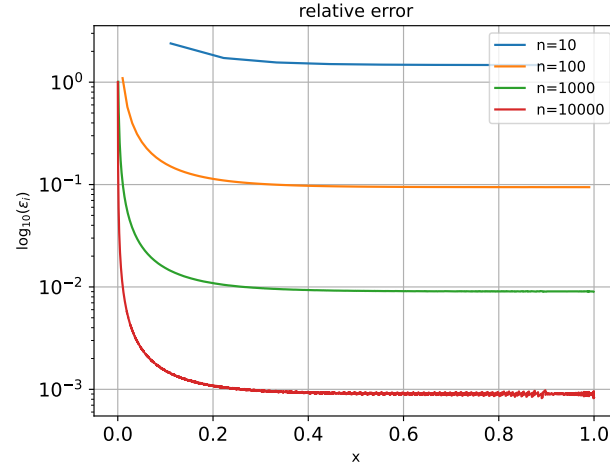


FIG. 4. The relative error of the general tridiagonal algorithm

Problem c

See FIG 5 for the plot for the table showing the maximum relative error. We see that for higher n the closer we get to 1.0, and from $n = 1000000$ the max relative error becomes 1.0.

n	max rel error
10	2.3903877077005538
100	1.0946543221364102
1000	1.0091303813999173
10000	1.0009115263620092
100000	1.000088892839682
1000000	1.0
10000000	1.0

FIG. 5. Table with the biggest relative error for each iteration

PROBLEM 9

Since the values of a, b, c never changes, we can just replace the arrays with a constant, saving us from repeatedly calculating $-(-1) \cdot \text{something}$.

Problem a

Algorithm 2 Algorithm for solving special tridiagonal matrix

arrays u , f , $temp$ of length n

$btemp = 2$

$u[1] = f[1] / 2$

for $i = 2, 3, \dots, n$ **do**

$temp[i] = -1 / btemp$

$btemp = b[i] + temp[i]$

$u[i] = (f[i] + u[i-1]) / btemp$

for $i = n-1, n-2, \dots, 1$ **do**

$u[i] -= temp[i+1] * u[i+1]$

Problem b

FLOPs: $1 + 4(n-1) + 2(n-1) = 1 + 6(n-1) = 6n - 5$

Problem c

See the function 'special_tridiag' in 'data_algorithms.cpp' in the github repository for the special algorithm.

PROBLEM 10

n	general	special
100	1.639e-06	7.334e-07
1000	1.6525e-05	7.2634e-06
10000	0.00016182	7.2397e-05
100000	0.001401	0.00073008
1000000	0.011985	0.011125
10000000	0.12067	0.11029

FIG. 6. A table showing the running time of the general and special algorithm for a given n

PROBLEM 11

LU decomposition has a complexity of $O(N^3)(+O(N^2))$ vs our algorithm that runs in $O(N)$. for $n = 10^5$ I would expect to:

1. Run out of memory, since you need to store $8 * N * N = 8 * 10^5 * 10^5 = 8 * 10^{10} \approx 80\text{GB}$.
2. To be very slow. The algorithm's O factor is two orders of magnitude larger, so probably around 100 times as long.