FYS3150 - project 1

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

PROBLEM 1

We have the one-dimensional Poisson equation

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

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

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

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

problem a)

See 'poisson_exact.cpp' and 'algorithms.cpp' in the github repository

problem b)

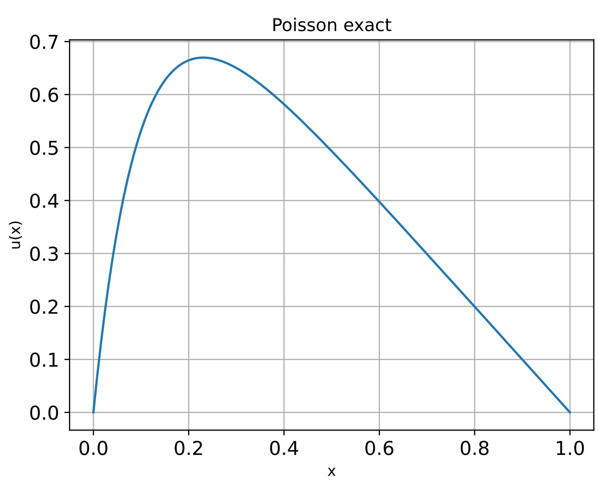

FIG. 1. A plot of the exact solution for the Poisson equation from 1 for $x \in [0, 1]$

PROBLEM 3

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

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

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

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

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

We then approximate and change the notation, $v_i \approx u_i$ and get

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

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

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

Equation 4 is a set of equations for every i

$$\begin{array}{llllll} i = 1 & -v_0 & 2v_1 & -v_2 & & = h^2 f_i \\ i = 2 & & -v_1 & 2v_2 & -v_3 & = h^2 f_2 \end{array}$$

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.

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

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

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

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

PROBLEM 5

Problem a

Since we're "dropping" 2 columns, $n = m - 2$

problem b

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

problem 6

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,...,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, ..., 1 do
    u[i] -= temp[i+1] * u[i+1]
```

problem b

FLOPs: $1 + 6(n-1) + 2(n-1) = 1 + 8(n-1) = 8n - 7$

PROBLEM 7

problem a

see 'general_tridiag.cpp' and 'algorithms.cpp' in the github repository

problem b

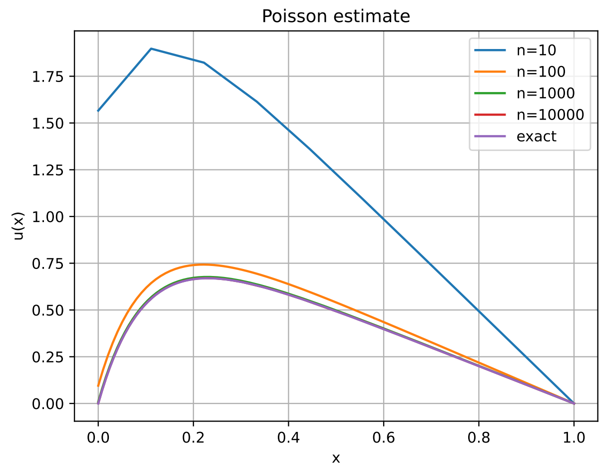

FIG. 2. Exact vs numerical comparison for the solution of equation 1

PROBLEM 8

problem a

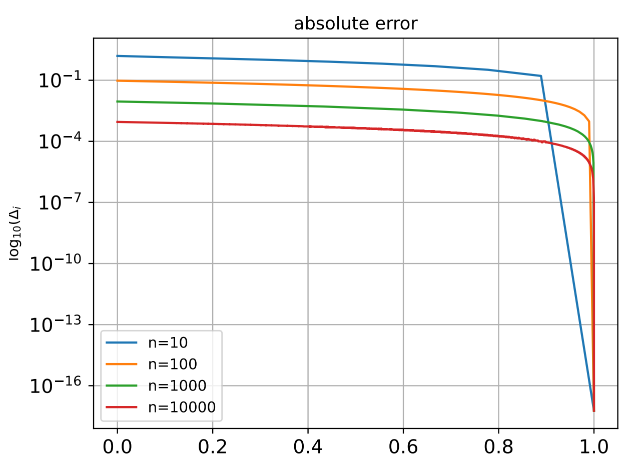

FIG. 3. The absolute error for the general tridiagonal alogrithm in log_{10}

problem b

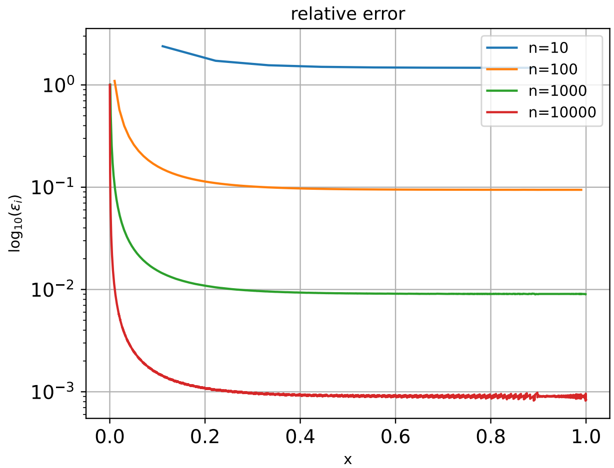

FIG. 4. The relative error of the general tridiagonal algorithm

problem c

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 constants, saving us from repeatedly calculating $-(-1) \cdot something$.

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,...,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, ..., 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

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 $8 * N * N = 8 * 10^5 * 10^5 = 8 * 10^{10} \approx 80$GB

2) to be very slow. The alogrithm's O factor is two orders of magnitude larger, so probably around 100 times as long.