FYS3150 Computational Physics - Project 1

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A look at different algorithms for solving a second-order differential equation with a known analytical solution, comparing both their speed and accuracy. Found that a specialized algorithm implemented in an efficient manner can speed up the computation significantly.

INTRODUCTION

THEORY, ALGORITHMS AND METHODS

We have second order inhomogeneous differential equation, Eqn. 1

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

With boundary conditions $\ddot{u}(x) = f(x)$, $u(0) = u(1) = 0$ and $x \in (0, 1)$.

If we let $f(x) = 100e^{-10x}$, then it can be shown analytically that the differential equation has a solution Eqn. 2

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

This problem can also be solved numerically by discretization. By the use of taylor expansions, it can be shown that there is a discrete, iterative solution in the form Eqn. 3 [1]

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

where $h = 1/(n + 1)$ is the step size for $n + 1$ points.

This problem can be written in the form

$$A\vec{v} = \vec{b} \tag{4}$$

Where A $\in R^{n\times n}$ is a tridiagonal matrix with diagonal elements 2 and -1 (Eqn. 5) and $\vec{b} = h^2(f_1, \ldots, f_n)$.

$$A = \begin{bmatrix} 2 & -1 & 0 & \ldots & \ldots & 0 \\ -1 & 2 & -1 & 0 & \ldots & 0 \\ 0 & -1 & 2 & -1 & \ldots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & -1 \\ \ldots & \ldots & \ldots & \ldots & -1 & 2 \end{bmatrix} \tag{5}$$

By matrix multiplication, when we multiply the i-th row of A by $\vec{v}$, we get

$$\begin{aligned} -1v_{i-1} + 2v_i - 1v_{i+1} &= -(v_{i+1} + v_{i-1} - 2v_i) \\ &= h^2 f_i \end{aligned} \tag{6}$$

Which is equivalent to the discretized differential equation Eqn. 3, showing that the differential equation can be solved as a linear algebra problem rather than iteratively.

RESULTS AND DISCUSSIONS

The implementation of the code discussed in the previous section can be found on my github: https://github.com/nicholaskarlsen/FYS3150. The benchmarks were tested on my computer without a running desktop environment etc, specifications listed in Table I

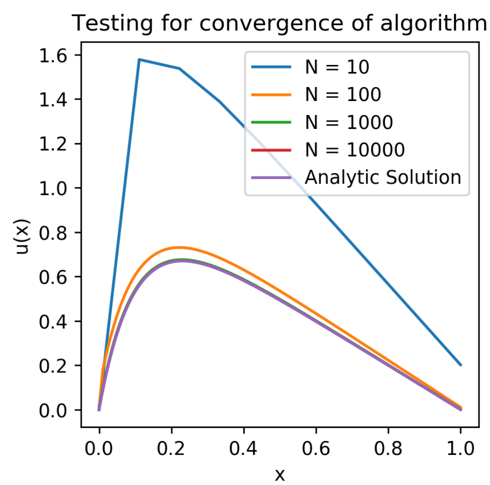

FIG. 1. A plot of the numeric solution for different N and the analytic solution.

CONCLUSIONS

[1] M. Hjorth-Jensen, Computational Physics - Lecture Notes 2015, (2015).

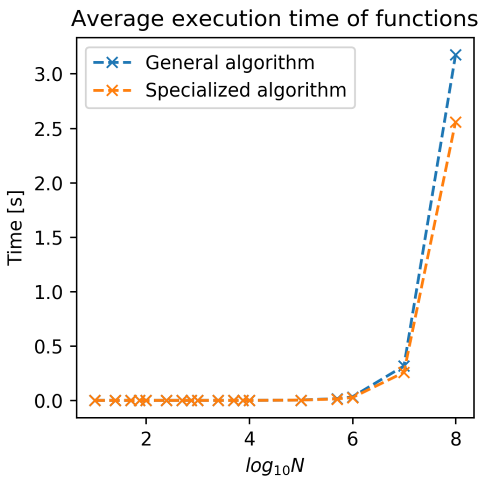

FIG. 2. Comparing the average execution time of 100 (or more) function calls for the general and specialized algorithm on my computer

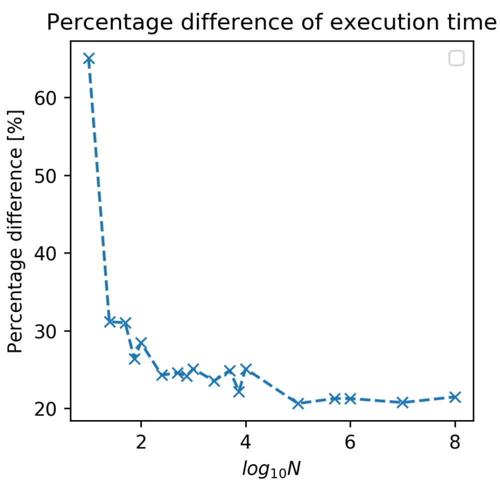

FIG. 3. Percentage difference between the execution times of the general and specialized algorithms on my computer

Appendix

TABLE I. PC Specifications

OS	Manjaro Linux
CPU	Intel i7-4790K (8) @ 4.400GHz
GPU	NVIDIA GeForce GTX 970
RAM	15969MiB

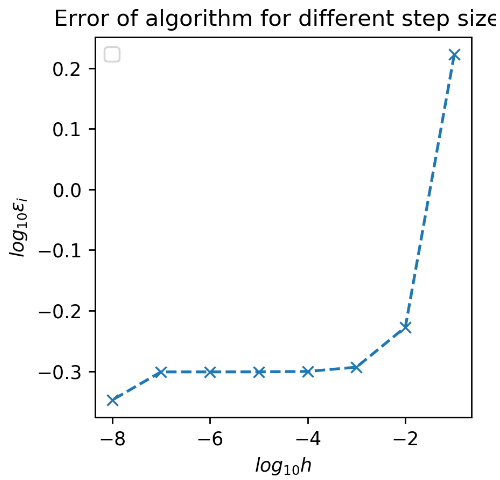

FIG. 4. Percentage difference between the execution times of the general and specialized algorithms on my computer