

Project 1

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Abstract

Introduction

Computing has had and still have an undeniable influence on science. has allowed scientist to explore everything from the tiniest scale of an atom,to tropical cyclones and galaxies. Therefore understanding the inner workings behind a computer program is critical in order to avoid unwanted errors. Errors which in the worst case can have catastrophic consequences [1].

Our aim is to investigate some of the common errors one might face if one doesn't think when developing code. To begin with we will look at a how to solve a second order differential equation, specifically the general one dimensional Poisson's equation (2).

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

Numerical differentiation

Computers operate in discrete steps, which means that variables are stored as discrete variables. A discrete variable defined over a particular range would have step length h between each value and can not represent any values in between. This means that how well a discrete variable would represent the continuous variable depends on the size of the step length. The step length h can either be set manually or it can be determined based on the start and end point of our particular range, $h = \frac{x_n - x_0}{n}$. Where n is the number of points we choose to have in our range. The shorter the step length in the discrete variable the better it will approximate the continuous variable.

The simplest way to compute the derivate numerically is to use what is called forward difference method eq.(2) or equivalently backward difference method (eq.3). If we include the limit as $\lim_{h \rightarrow 0}$ we obtain the classic definition of the derivate.

$$f'(x) \approx \frac{f(x + h) - f(x)}{h} \quad (2)$$

$$f'(x) \approx \frac{f(x - h) + f(x)}{h} \quad (3)$$

Since numerical differentiation always will give an approximation of the derivate, we would like to quantify our error. The error can be derived if we do a taylor series expansion of the $f(x + h)$ term in around x .

$$f(x + h) = f(x) + h'f(x) + \frac{h^2 f''(x)}{2} + \frac{h^3 f'''(x)}{6} + \dots \quad (4)$$

If we next insert this taylor expansion into eq.(4) we get:

$$f'(x) = f'(x) + \frac{hf''(x)}{2} + \frac{h^2f'''(x)}{6} + \dots \quad (5)$$

Our approximation of the derivate includes $f'(x)$ and some terms which are proportional to $h, h^2, h^3 \dots$ and since h is assumed to be small the h terms would dominate. The error is said to be of the order h .

To get a numerical scheme for the second derivate we would just take the derivate of eq. (2) except for a slight modification. Instead of looking at $f''(x) \approx \frac{f'(x+h)-f'(x)}{h}$ we would use $f''(x) \approx \frac{f'(x)-f'(x-h)}{h}$, which are equivalent to each other see. [2].

$$f''(x) \approx \frac{f(x+h) - f(x) - f(x-h+h) + f(x-h)}{h^2} \quad (6)$$

Then after a bit of a clean up we get an approximation for the second order derivate (eq. (7)).

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \quad (7)$$

Then to quantify the error we proceed as for the first order derivate, by expanding $f(x+h)$ and $f(x-h)$.

$$f(x-h) = f(x) - hf'(x) + \frac{h^2f''(x)}{2} - \frac{h^3f'''(x)}{6} \dots \quad (8)$$

Next we substitute the two taylor expansion eq. (8) and eq. (4) into the expression for second order derivate eq. (7).

$$f''(x) \approx f''(x) + \frac{h^2f^{(4)}(x)}{4!} + \frac{h^4f^{(6)}(x)}{6!} + \dots \quad (9)$$

Then we see that leading error term is for the second derivate is $\mathcal{O}(h^2)$.

Methods

Building upon the previously described concepts of numerical derivatives, we will now describe how to solve our differential equation eq. (1) numerically by rewriting it as a set of linear equations.

Explicitly, we will solve the differential equation:

$$-u''(x) = f(x), \quad x \in (0, 1), \quad u(0) = u(1) = 0$$

We will define the discrete approximation to $u(x)$ as v_i with grid points $x_i = ih$ in the range from $x_0 = 0$ to $x_{n+1} = 1$, and the step length is defined as $h = 1/(n + 1)$. The boundary conditions is $v_0 = 0$ and $v_{n+1} = 0$. The second derivate we approximate according to eq. (7) and also introducing the short-hand notation we get eq. (10).

$$g_i = -\frac{v_{i-1} - 2v_i + v_{i+1}}{h^2} \quad \text{for } i = 1, 2, 3, \dots, n \quad (10)$$

To see how eq. (10) can be represented as matrix equation, we will first multiply each side by h^2 .

$$v_{i-1} - 2v_i + v_{i+1} = g_i h^2, \quad \tilde{g}_i = g_i h^2$$

Next we represent the v_i 's and the \tilde{g}_i 's as a vectors,

$$\mathbf{v} = [v_1, v_2, v_3, \dots, v_n], \quad \tilde{\mathbf{g}} = [\tilde{g}_1, \tilde{g}_2, \tilde{g}_3, \dots, \tilde{g}_n]$$

Then if we transpose our two vectors we only need to find the $n \times n$ matrix \mathbf{A} and our matrix equation is complete. The matrix \mathbf{A} would in our case look like this.

$$\mathbf{A} = \begin{bmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & & -1 & 2 & -1 \\ 0 & \dots & & 0 & -1 & 2 \end{bmatrix}$$

It is easy to verify that $\mathbf{Av} = \tilde{\mathbf{g}}$ would give us eq. (10) by doing the matrix multiplication.

Thomas Algorithm

Results

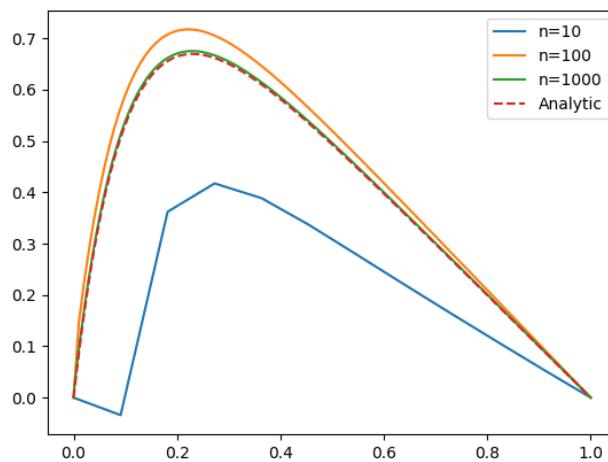


Figure 1: Comparison of analytic solution and numerical approximations

$\log_{10}(h)$	max(relative error)
-1.04	2.82e-02
-2.00	-1.50e-01
-3.00	-2.21e-02
-4.00	-3.24e-03
-5.00	-4.33e-04
-6.00	-5.43e-05

Table 1: Maximum relative error between analytic and numeric solution.

After running the thomas and toeplitz algorithm on matrixes from 10×10 to 1000000×1000000 , and the lower/upper decomposition + backward substitution (LU) on matrixes from 10×10 to 1000×1000 ten times and taking the average we got the results in table 3.

To see how the algorithm time for our different methods scales with n we divide all timings with n (table 3). Both the thomas and toeplitz algorithm times (normalized by n) are of the same order, as was expected from the counting of flops. The times for LU show an increase of to orders of magnitude for each

n	thomas	toeplitz	lu
10	2.560e-05	2.670e-05	3.580e-04
100	2.550e-04	2.160e-04	1.450e-01
1000	4.090e-03	1.220e-03	1.230e+02
10000	2.600e-02	1.170e-02	
100000	2.590e-01	1.220e-01	
1000000	2.680e+00	1.280e+00	

Table 2: Summary of algorithm times.

magnitude increase in n. This is consistent with our expectations of the LU algorithm time being proportional to n^3 .

n	thomas	toeplitz	lu
10	2.560e-06	2.670e-06	3.580e-05
100	2.550e-06	2.160e-06	1.450e-03
1000	4.090e-06	1.220e-06	1.230e-01
10000	2.600e-06	1.170e-06	
100000	2.590e-06	1.220e-06	
1000000	2.680e-06	1.280e-06	

Table 3: Algorithm times divided by n.

Comparing the algorithm times of thomas and toeplitz (table 4) we see they are the same order of magnitude. Theoretically we would expect the toeplitz algorithm to be $\frac{9FLOPS}{4FLOPS} \approx 2.25$ times as fast as toeplitz, and our results for larger values of n are quite close.

n	thomas/toeplitz	lu/toeplitz
10	9.588e-01	1.341e+01
100	1.181e+00	6.713e+02
1000	3.352e+00	1.008e+05
10000	2.222e+00	
100000	2.123e+00	
1000000	2.094e+00	

Table 4: Algorithm times of thomas divided by that of toeplitz.

References

1. Arnold, D. N. *The sinking of the Sleipner A offshore platform* <http://www-users.math.umn.edu/~arnold/disasters/sleipner.html>. (accessed: 01.09.2019).
2. Scott, B. M. *Second derivative formula derivation* <https://math.stackexchange.com/q/210269>. (accessed: 05.09.2019).