

Homework 2

due January 31 2017, 23:59

Task 1: Machine Epsilon

In general a computer stores a real number in the following way

$$x = (-1)^s \cdot (0.a_1a_2\dots a_t) \cdot \beta^e = (-1)^s \cdot m \cdot \beta^{e-t}, \quad a_1 \neq 0$$

where s is either 0 or 1, β (a positive integer larger than or equal to 2) is the *basis* adopted by the specific computer at hand, m is an integer called *mantissa* whose length t is the maximum number of digits a_i (with $0 \leq a_i \leq \beta - 1$) that are stored, and e is an integral number called the *exponent*. The numbers given in this form are called floating-point numbers, since the position of the decimal point is not fixed. The digits $a_1a_2\dots a_p$ (with $p \leq t$) are called the p first significant digits of x . The accuracy with which floating-point numbers are stored depends then on β and t , and so does the amount of memory required to store them. For example, double precision real numbers are stored in registers of 8 Bytes: the sign s is stored in 1 bit, the exponent e in 11 bits, and the mantissa m in 52 bits. Note that, although there are 52 bits for m , we can count $t = 53$ digits when $\beta = 2$. As a matter of fact, since the first digit a_1 of every floating point number must be different from 0, when $\beta = 2$ it is worthless to store it as it must necessarily be 1. A *round-off error* is inevitably generated whenever a real number $x \neq 0$ is replaced by its floating-point representative x_{num} , this error is always limited by

$$\frac{|x - x_{\text{num}}|}{|x|} \leq \frac{1}{2}\varepsilon,$$

where $\varepsilon = \beta^{1-t}$, called *machine epsilon*.

The following code can be used in MATLAB to compute ε .

```
numprec=double(1.0); % Define 1.0 with double precision
numprec=single(1.0); % Define 1.0 with single precision
while(1 < 1 + numprec)
    numprec=numprec*0.5;
end
numprec=numprec*2
```

- Determine ε using the above program, both for single and double precision.
- Explain in detail what the code does. Why do we consider addition to 1?
- Explain the difference between single and double precision. How many Bytes are used to store a single precision number? How many for the mantissa?

Task 2: Round-off Error

In this exercise, the errors involved in the numerical approximation of derivatives are examined. Using central finite differences the derivative of a function $f(x)$ can be approximated as:

$$f'(x) \approx f'_{\text{num}}(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} \quad (1)$$

- a) Compute, numerically, the relative discretization error of the derivative of the function $f(x) = \frac{1}{1+x} + x$ using equation (1). The relative discretization error is given by:

$$\xi_d = \frac{|f'(x) - f'_{\text{num}}(x)|}{|f'(x)|}, \quad (2)$$

where $f'(x)$ is the analytical derivative of $f(x)$. Compute ξ_d at $x = 2$ for different step-sizes $\Delta x \in [10^{-20}, 1]$. Use both single and double precision for the calculation and present the results in a double logarithmic plot¹ (ξ_d vs. Δx). Remember that *all* variables used here should be defined as double or single precision as in Task 1.

- b) The absolute propagation error ξ_p of an arithmetic operation \circ ($+$, $-$, \times or $/$) between two numbers a_1 and a_2 can be evaluated as: $a_1 \circ a_2 - a_{1,\text{num}} \circ a_{2,\text{num}}$, where $(\cdot)_{\text{num}}$ is the machine representation of the respective number.

Show that the propagation error of the addition of two positive numbers a_1 and a_2 is given by

$$\xi_{p,\text{add}} = \frac{a_1}{a_1 + a_2} \varepsilon_{a_1} + \frac{a_2}{a_1 + a_2} \varepsilon_{a_2}, \quad (3)$$

where $\varepsilon_{a_j} := (a_j - a_{j,\text{num}})/a_j$ is the machine accuracy on the quantity $a_{j,\text{num}}$.

A general formula for the propagation error for a function $g(a_1, a_2, \dots, a_n)$ representing multiple arithmetic operations is given by:

$$\xi_p = \sum_{j=1}^n \left| \frac{a_j}{g} \frac{\partial g}{\partial a_j} \right| \varepsilon_{a_j}, \quad (4)$$

Show that when $g = a_1 + a_2$ this formula results in equation (3).

- c) Show that, when using the proposed central differences approximation, the relative discretization error (equation (2)) is given by:

$$\xi_d \approx \frac{\Delta x^2 |f'''(x)|}{6|f'(x)|}$$

(Hint: Taylor expansion)

and that the propagation error (equation (4)) is given by:

$$\xi_p \approx \frac{|f(x)|\varepsilon}{|f'(x)|\Delta x}$$

where ε is the machine accuracy. Find, analytically, the value of Δx that minimizes the total error

$$\xi_{\text{tot}} = \xi_d + \xi_p.$$

Plot ξ_d , ξ_p and ξ_{tot} together with the results from part a).

¹In MATLAB double logarithmic plots are obtained by the function `loglog()`.

Task 3 : Discretization in time

In this problem the stability and convergence order of three numerical time discretization methods is examined. Consider the first order, linear, test equation (the Dahlquist equation)

$$\begin{cases} u'(t) = f(u) = \lambda u(t), & 0 < t \leq T, \\ u(0) = 1 \end{cases} \quad (5)$$

where $\lambda = \lambda_{\Re} + i\lambda_{\Im} \in \mathbb{C}$. The time interval $[0, T]$ is discretized into N equally spaced parts: $t_n = n\Delta t$, $n = 0, 1, \dots, N$, where Δt is the step-size. The following numerical methods should be used:

- explicit Euler

$$u^{n+1} - u^n = \Delta t f(u^n)$$

- implicit Euler

$$u^{n+1} - u^n = \Delta t f(u^{n+1})$$

- Crank-Nicolson

$$u^{n+1} - u^n = \frac{1}{2} \Delta t [f(u^{n+1}) + f(u^n)]$$

where $u^n := u(t_n)$.

- Solve the system (5) analytically (by hand) to obtain the exact solution $u = u_{ex}$.
- For $\lambda = -\sqrt{3}/2 + i\pi$ and for the five cases $N = 20, 40, 50, 100$, and 200 , compute the numerical solution iteratively until $T = 10$ for all the three methods. Plot the real part of the solutions together with the exact solution for each value of N . What do you observe?
- Now, consider $\lambda \in \mathbb{R}$. For each of the three considered schemes: (i) derive the expression of the amplification factor $G(z)$, where $z := \lambda\Delta t$; (ii) calculate $\lim_{z \rightarrow -\infty} G(z)$; (iii) plot $G(z)$ as a function of z together with the result for the exact amplification over the interval $z \in [-10, 0.5]$. Discuss the performance of the schemes in the limits $z \rightarrow -\infty$ and $z \rightarrow 0$. Also, answer: why is the imaginary part of λ irrelevant for this analysis?
- For $\lambda = -\sqrt{3}/2 + i$, first do as in b) and explain the differences. Then, for each method, at a fixed time (chose $t = 3$) compute and plot the error $|u_{ex} - u_{num}|$ as a function of N in a double logarithmic plot and estimate the order of accuracy by considering the slope of the curve. (Hint: $\log(x^p) = p \log(x)$.)
- Based this task, discuss the usefulness, stability and accuracy of the methods.