MA579H Scientific Computing

Lecture 1: Introduction

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Course Logistics

Instructor: Rafikul Alam

Lab Teaching Assistant: Dr. Prince Kanhya

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I will post lecture slides, homework and programming assignments on Microsoft Teams.

Course Syllabus

Definition and sources of errors; Solutions of nonlinear equations; Bisection method, Newton's method and its variants, fixed point iterations, convergence analysis; Newton's method for non-linear systems;

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Textbooks:

- D. Kincaid and W. Cheney, Numerical Mathematics and Computing, 7th Edn., Cengage, 2013.
- K. E. Atkinson, Introduction to Numerical Analysis, 2nd Edn., John Wiley, 1989.
- Timothy Sauer, Numerical Analysis, 3rd Edition, Pearson, 2018.

Assessment

Grading will be based on continuous assessments.

- Quiz: 30 %
- End/Mid semester examination: 60 %
- Assignment/Viva: 10 %

Lab experiments will be assessed as a part of MA581 Numerical Computations Lab. Grading will be based on assignments (20 %), mid semester examination (30 %) and end semester examination (50 %).

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- Solution of ordinary and partial differential equations
- Solution of linear and nonlinear algebraic equations

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Modified method: Clever use of the formula yields $(x_1 x_2 = c/a)$

$$x_1 = -\frac{b + \mathrm{sign}(b)\sqrt{b^2 - 4ac}}{2a}, \quad x_2 = \frac{c}{a x_1}$$

Example

Solve $10^{-3}x^2 + 10^7 x + 3 = 0$

$$x_1 = \frac{-10^7 - \sqrt{10^{14} - 12 \times 10^{-3}}}{2 \times 10^{-3}} \approx -1.0 \times 10^{10}$$

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Problem: Compute $\dfrac{e^x - 1 - x}{x^2}$ for $x \approx 0$. THINK.

Analysis

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- stability (reliability) of numerical methods (algorithms)
- efficiency of numerical methods (i.e., complexity of algorithms),
- the effect of finite precision arithmetic upon algorithms, and
- approximation errors and accuracy of solutions.

Example 1

Let $f : \mathbb{R} \longrightarrow \mathbb{R}$ be differentiable. Then $f'(x) := \lim_{h \to 0} \dfrac{f(x+h) - f(x)}{h}$.

Define $D_h f(x) := \dfrac{f(x+h) - f(x)}{h}$ and $E(x, h) := |f'(x) - D_h f(x)|$.

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Since $\lim_{h \to 0} D_h f(x) = f'(x)$, in theory,

$$|h| \text{ small } \implies E(x, h) \text{ is small.}$$

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For $f(x) = e^x$, we plot $E(0, h)$ as a function of h.

The plot shows that $|E(0, h)|$ decreases as h decreases to certain $h_{\min}$ and then starts increasing when $h < h_{\min}$ further decreases to 0.

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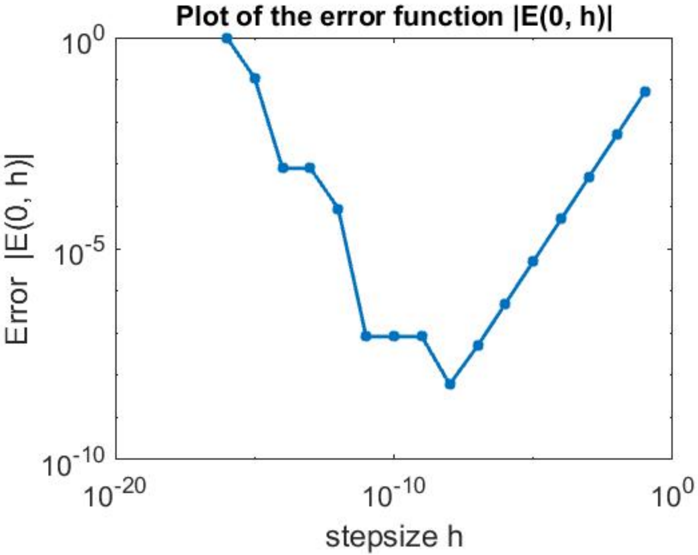
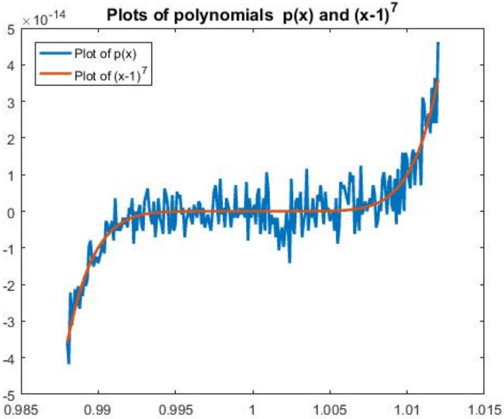
How do you explain this behavior of $|E(0, h)|$?

Example 1


Plot of the error function |E(0, h)|
Error |E(0, h)|
10^{0}
10^{-5}
10^{-10}
10^{-20}
10^{-10}
10^{0}
stepsize h

Example 2

Let $p(x) = x^7 - 7x^6 + 21x^5 - 35x^4 + 35x^3 - 21x^2 + 7x - 1 = (x-1)^7$.



Does the plot look like a polynomial? What explains this behaviour?

Implementation

The implementation of numerical methods (algorithms) deals with development of efficient, reliable and portable software for solving mathematical problems that arise in science and engineering.

Outline of topics

- Finite precision arithmetic and propagation errors
- Polynomial interpolation

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- Numerical integration and differentiation
- Solution of nonlinear equations
- Solution of initial value ordinary differential equations

Learning outcome

This course will equip you with rigorous knowledge of the core topics, namely,

- root-finding techniques
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- solution of initial value problem (ODEs)

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Also, you will learn how to use MATLAB to implement these algorithms and adapt the codes for more general problems.

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