Numerical Methods KOM2722-AVE3842

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Syllabus

Texts:

- An Introduction to Numerical Methods and Analysis, J. F. Epperson, Wiley, 2002
- Applied Numerical Methods with MATLAB, S.C. Chapra, 2012, McGrow-Hill

Lecture Notes

- We will use lecture notes of Asst. Prof. Birol Erol and Asst. Prof. Bahadır Çatalbaş prepared from textbooks.
- Lecture slides will be shared with students.

Grading:

- 60% Midterm
- 40% Final

Course Coverage

1. Motivation, Basic Tools of Calculus, Simple Approximations
2. Horner’s Rule, Euler’s Method
3. Linear Interpolation
4. Root Finding Methods (The Bisection Method, Newton’s Method)
5. Root Finding Methods (The Secant Method, Fixed Point Iteration, etc.)
6. Root Finding Methods (Other techniques)
7. Lagrange Interpolation
8. Midterm Exam

Course Coverage

9. Newton Interpolation and Divided Differences
10. Piecewise Polynomial Interpolation and Introduction to the Splines
11. Least Squares Methods in Approximation
12. Numerical Integration
13. Numerical Methods for Ordinary Differential Equations(Initial Value Problem and Euler Method)
14. Linear Equation Systems and Gauss Elimination, LU(Lower-Upper) Factorization
15. Final

Aim of Course

- Formulization and analytical thinking
- Ability to apply knowledge of mathematics, science and engineering learning design
- Solve complex problems using computers

Importance of Numerical Methods

- Powerful problem solving tools for
  - Large system of equations
  - Solution of nonlinear equations
- Efficient way of learning computer logic and programming
- Learn to how math is employed in engineering

Problem-Model-Solution

- In engineering, we propose mathematical models for problems.
- After that, we apply the analytical or numerical method to end up with solutions.

Analytical Methods:

Exact solutions to to problems. Hovewer it may not be computationally feasible to obtain it.

Numerical Methods:

Since analytical solution may not be exist or even if it exists, it may not be computationally feasible to calculate we benefit from methods called numerical methods.

Here we need some approximations so then we decide and have “close enough” solution.

Some examples are integration, differentiation, optimization etc.

Problem-Model-Solution

Mathematical models are utilized to understand and solve real world problems such as

-Energy -Environmental Issue -Transportation -Financial Problems

To solve these problems using approximations and obtain “close-enough” results compared to analytical solution, errors are added to our solution and we know it…

Accuracy:

Refers to the closeness of a value to the reference standard.

There will be an error, so it is needed to understand how to handle this error.

Efficiency:

Does the algorithm take an inordinate amount of computer time?

* There is a trade of between **accuracy** and **efficiency**. They compete so to make an algorithm more accurate usually make it more costly and less efficient.

Stability:

Does the method produce similar results for similar data?

If we change data by a small amount, do we get big differences? If so, the method is unstable.

Basic Tools of Calculus
Taylor's Theorem

Provides an approximation of $(n+1)$ times differentiable function around a given point.

Suppose that we are working on a function f(x) that is continuous and has $(n+1)$ continious derivatives on interval $(a, b]$.

Theorem (Taylor's Theorem with Remainder):

Let $f(x)$ have $n+1$ continuous derivatives on $(a, b]$ for some $n \geq 0$ and let $x, x_0 \in [a,\ b]$, then

$$f(x) = p_n(x) + R_n(x)$$

$$p_n(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)(x-x_0)^2}{2!} + \cdots = \sum_{k=0}^{n} \frac{(x-x_0)^k}{k!} f^{(k)}_{(x_0)}$$

The remainder

$$R_n(x) = \frac{1}{n!}\int_{x_0}^{x} (x-t)^n\, f^{(n+1)}(t)dt$$

*Every continuous function can be approximated by a polynomial of order n.

*Allow us to replace/obtain, in a computational setting, a much simple problem.

The remainder, the error term,

$$R_n(x) = \frac{(x-x_0)^{n+1}}{(n+1)!} f^{(n+1)}(c) for\ some\ c\ between\ x_0\ and\ x$$

$$and$$

$$\lim_{n \to \infty} R_n(x) = 0$$

Taylor's series for $x_0 = 0$ is called as Maclaurin series

<u>Example:</u> $f(x) = e^x$, find n^{th} order Taylor series expansion of $f(x)$ around $x = 0$

$$f^{(k)}(0) = 1$$

$$e^x = 1 + \underbrace{x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots + \frac{1}{n!}x^n}_{p_n(x)} + \underbrace{\frac{1}{(n+1)!}x^{n+1}e^{c_x}}_{R_n(x)}$$

$R_n(x)$, remainder c_x is an unknown point between x and 0.

Example: $f(x) = \ln(1 + x)$, find the Taylor series expansion of $f(x)$ around $x = 0$

$$f(x) = \ln(1 + x) \;\; \text{=>} \; f(0) = 0$$

$$f'(x) = \frac{1}{1+x} \;\; \text{=>} \; f'(0) = 1$$

$$f''(x) = \frac{-1}{(1+x)^2} \; \text{=>} \; f''(0) = 2$$

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \cdots = \sum_{n=0}^{\infty}(-1)^n \frac{x^{n+1}}{n+1}$$

Example: $f(x) = \sin(x)$, find the Taylor series expansion of $f(x)$ around $x = 0$

$f(x) = \sin(x)$ => $f(0) = 0$

$f'(x) = \cos(x)$ => $f'(0) = 1$

$f''(x) = -\sin(x)$ => $f''(0) = 0$

$f'''(x) = -cos(x)$ => $f'''(0) = -1$

$$\sin(x) = x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 + \cdots + \frac{(-1)^n}{(2n+1)!}x^{2n+1} + \frac{(-1)^{n+1}}{(2n+3)!}x^{2n+3}\cos(c_x)$$

$$= \sum_{k=0}^{n} \frac{(-1)^k}{(2k+1)!}x^{2k+1} + R_n(x)$$

$$\cos(x) = 1 - \frac{1}{2!}x^2 + \frac{1}{4!}x^4 + \cdots + \frac{(-1)^n}{(2n)!}x^{2n} + \frac{(-1)^{n+1}}{(2n+2)!}x^{2n+2}\cos(c_x)$$

$$= \sum_{k=0}^{n} \frac{(-1)^k}{(2k)!}x^{2k} + R_n(x)$$

Taylor's Theorem an approximation and an error estimate provides

Considering the problem of approximating the exponential function on the interval $[-1, 1]$

$$e^x = \underbrace{1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots + \frac{1}{n!}x^n}_{p_n(x)\ \text{Polynomial}} + \underbrace{\frac{1}{(n+1)!}x^{n+1}e^{c_x}}_{R_n(x),\ \text{remainder}}$$

c_x is an unknown point between x and 0.

Without lost of generality x can be any point in [-1, 1] then

c_x can be any point in [-1, 1]

For simplicity, let's denote polynomial by $p_n(x)$ and remainder by $R_n(x)$, so that the equation:

$$\mathrm{e}^x = p_n(x) + R_n(x)$$

Suppose that we want this approximation to be accurate within 10^{-6} absolute error. i.e.,

$|\mathrm{e}^x - p_n(x)| \leq 10^{-6}$ for all x in the interval $[-1, 1]$.

$|\mathrm{e}^x - p_n(x)| = |R_n(x)| \leq 10^{-6}$, if we make $|R_n(x)| \leq 10^{-6}$ the absolute error in approximation will be less that 10^{-6}.

In other words, we need make the **upper bound** less than 10^{-6}.

$$|R_n(x)| = \frac{|x^{n+1}e^{cx}|}{(n+1)!} = \frac{|x|^{n+1}e^{cx}}{(n+1)!}$$ (Note that: $e^z > 0$ <u>for all z.)</u>

$\leq \frac{e^{cx}}{(n+1)!}$, because |x| $\leq$ 1 for all x ∈ [-1, 1]

$\leq \frac{e}{(n+1)!}$, because $\mathrm{e}^{cx} \leq e$ for all x ∈ [-1, 1]

So that, if we find n such that $\frac{e}{(n+1)!} \leq 10^{-6}$ then we will have $|e^x - p_n(x)| = |R_n(x)| \leq 10^{-6}$.

$n = 9$ satisfies the desired accuracy.

The error defined as ($|\mathrm{e}^x - p_n(x)|$) increases and accuracy of approximation decreases as we get away from the interval $[-1,\ 1]$. This is expected since the Taylor polynomial is constructed to match function $f(x)$ and its first derivatives at $x = x_0$, so $p_n(x)$ is a good approximation to $f(x)$ only when x is near to x_0.

Example: Find the minimum order of Taylor series expansion for $f(x) = \sin(\pi x)$ to be accurate within 10^{-4} absolute error for all $x \in [-\frac{1}{2}, \frac{1}{2}]$ using $x_0 = 0$.

$$p_n(x) = \pi x - \frac{1}{6}\pi^3 x^3 + \frac{1}{120}\pi^5 x^5 + \cdots + (-1)^n \frac{1}{(2n+1)!}\pi^{2n+1} x^{2n+1}$$

$$R_n(x) = (-1)^{n+1} \frac{1}{(2n+3)!}\pi^{2n+3} x^{2n+3} \cos(c_x)$$

The error

$|f(x) - p_n(x)| = |R_n(x)| = \frac{1}{(2n+3)!}(\pi x)^{2n+3} |\cos(c_x)|$, where c_x is between x and 0. It can be bounded $c_x \in [-\frac{1}{2}, \frac{1}{2}]$ interval

$$|R_n(x)| = \frac{|\pi x|^{2n+3}}{(2n+3)} |\cos(c_x)| \le \frac{|\pi x|^{2n+3}}{(2n+3)}$$

By using calculator

$|R_4(x)| \le 0.3599x10^{-5}$, $|R_3(x)| \le 0.1604x10^{-3}$, $n = 4$ achieves desired accuracy

$$p_4(x) = \pi x - \frac{1}{6}\pi^3 x^3 + \frac{1}{120}\pi^5 x^5 - \frac{1}{5040}\pi^7 x^7 + \frac{1}{362880}\pi^9 x^9$$

Consider the problem of expanding $f(x+h)$ in a Taylor Series, about point $x_0 = x$

Here h is generally considered to be small parameter,

$$f(x+h) = f(x) + \big((x+h)-x\big)f'(x) + \tfrac{1}{2}\big((x+h)-x\big)^2 f''(x)$$

$$+ \cdots + \tfrac{1}{n!}\big((x+h)-x\big)^n f^{(n)}(x) + \tfrac{1}{(n+1)!}\big((x+h)-x\big)^{(n+1)} f^{(n+1)}(\zeta)$$

$$= f(x) + hf'(x) + \tfrac{1}{2}h^2 f''(x) + \cdots + \tfrac{1}{n!}h^n f^n(x) +$$

$$+ \tfrac{1}{(n+1)!}h^{n+1} f^{(n+1)}(\zeta)$$

This kind of expansion will be useful time and again in our studies.