

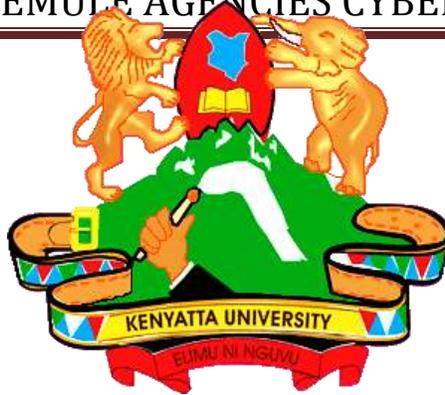


SMA 330 Module 240909 094043

Numerical Analysis 1 (Kenyatta University)



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KENYATTA UNIVERSITY

DIGITAL SCHOOL OF VIRTUAL AND OPEN LEARNING

SCHOOL OF PURE & APPLIED SCIENCES

DEPARTMENT OF MATHEMATICS

UNIT CODE & NAME: SMA 330 NUMERICAL ANALYSIS I

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INTRODUCTION

Numerical Analysis is the study of methods (algorithms) that use numerical approximation (as opposed to general symbolic manipulations) for the problems of Continuous Mathematics (as distinguished from Discrete Mathematics). Numerical methods are methods for solving problems numerically (in terms of numbers) on a computer, a calculator or by hand. Numerical analysis naturally finds applications in all fields of engineering and physical sciences but in the current world the life sciences and even arts have adopted elements of scientific computing. Much research is going on in improving existing methods and investigating stability or accuracy of methods.

The purpose of this module is to introduce the learners to various numerical methods such as interpolation, error analysis, differentiation, integration and iteration. The module has six lectures. Lecture 1 provides an introduction to errors and machine computation. In lecture 2, polynomial functions are discussed while lecture 3 contains the derivation of interpolating polynomials and approximating functions. In lecture 4 Numerical differentiation is discussed while lecture 5 discusses different methods of numerical integration. Lecture 6 contains direct and iteration methods for solution of non-linear equations. From these lectures it should be noted that the overall goal of Numerical analysis is the design and analysis of techniques to give approximate but accurate solutions of problems.



2. OBJECTIVES

By the end of this course the learner should be able to:

1. To solve complex numerical problems using only the simple operations of arithmetic.
2. To develop and evaluate methods (algorithms) for computing numerical results from given data.



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LECTURE ONE**ERRORS AND APPROXIMATIONS IN NUMERICAL COMPUTATIONS****1.1 INTRODUCTION**

Numerical analysis involves the development and evaluation of methods for computing required numerical results from given numerical data. In numerical computations, errors and approximations are always involved and hence the result is approximate and very near to the true value. In this lesson possibilities of error occurrence and measures to safeguard against the errors are discussed.

Rarely will input information be exact since it ordinary comes from measurement devices of some sort. The quantity true value minus approximate value is called the error.

**1.2 LECTURE OBJECTIVES**

By the end of this lecture the learner should be able to:

- i) Define and calculate round off and truncation errors.**
- ii) Identify measures take to minimize round off errors**
- iii) Define and calculate absolute, relative and percentage errors.**
- iv) Calculate propagated errors with reference to numerical computations.**

1.3 Round off and truncation errors

Round off errors arise because it is impossible to represent all real numbers exactly on a machine (computer) with finite memory. It involves dropping out decimal points or significant figures and can be done by chopping or truncating and by symmetric rounding.



ACTIVITIES

The table below gives certain real numbers rounded off using different conditions.

Real No.	Round off to 4sf	Round off to 4.3dp	Chopped to 4s
$\frac{4}{3} = 1.3333$	1.333	1.3333	1.333
$\frac{1}{30} = 0.03333$	0.03333	0.0333	0.03333
$\frac{2}{3} = 0.6666$	0.6667	0.6667	0.6666
$\pi = 3.14159$	3.142	3.1416	3.141

When rounding to n dp the error introduced should be $error < 10^{-n}$

Example $\pi = 3.14159$ to 4dp is 3.1416.

$$error = 3.1416 - 3.14159 = 10^{-4}$$

1.4 Absolute and Relative error

Let x^r be an approximate number to an exact number x .

Absolute error is the absolute difference between the exact number x and the approximate number x^r .

$$cabs = |x - x^r|$$

Let Δx be such that $cabs = |x - x^r| = \Delta x$, where $\Delta x \rightarrow$ upper bound



ACTIVITIES

Activity 1

$x^r = 2.4$ correct to one decimal place,

Approximate $XE(2.35, 2.45)$, that is $2.35 \leq 2.45$.

$$2.35 - 2.4 \leq x - x^r \leq 2.45 - 2.4$$

$$|-0.05| \leq |x - x^r| \leq |0.05|$$

$$Cabs = 0.05 \text{ or } 5.0 \times 10^{-2}$$

Activity 2

Let $x^r = -10.788$ correct to 3D.

Approximate $XE[-10.7885, -10.7875]$

$$-10.7885 \leq x \leq -10.7875$$

$$-10.7885 + 10.788 \leq x - x^r \leq -10.7875 + 10.788$$

$$Cabs = x^r = 0.0005 = .5 \times 10^{-3}$$

In general, if a number is correct to $n\Delta$

$$\text{Max } cabs = .5 \times 10^{-n}$$

$$cabs = .5 \times 10^{-n}$$

e.g. 8.35678, $cabs \leq .5 \times 10^{-5}$

Relative error (e_r)

Relative error is defined as $\frac{cabs \text{ in } X^r}{|X|}$

$$= \frac{|X - X^r|}{|X|}$$

$$\text{Max } e_r \text{ in } x^r = \frac{\Delta X}{|X|}$$

$$\text{Let } X = X + X^r - x^r - (X^r - X)$$

$$|X| = |X|(X^r - (X^r - X))$$

$$|X| \geq |X^r| - |X^r - X|$$

$$|X| \geq |X^r| - cabs$$

$$\frac{1}{|X|} \leq \frac{1}{|X^r| - cabs}$$

$$\frac{cabs}{|X|} \leq \frac{cabs}{|X^r| - cabs}$$

$$e_r \leq \frac{cabs}{|X^r| - cabs}$$

$$\text{Max } e_r = \frac{cabs}{|X^r|} \text{ where } |X^r| \gg cabs$$

Example

- a) If $P = 0.3000 \times 10^1$ and $P^r = 0.3100 \times 10^1$ absolute error is 0.1
Relative error 0.3333×10^{-3}
- b) If $P = 0.3000 \times 10^{-3}$ and $P^r = 0.3100 \times 10^{-3}$
 $cabs = 0.3000 \times 10^{-4}$, $e_r = 0.3333 \times 10^{-1}$
- c) If $P = 0.3000 \times 10^{-4}$ and $P^r = 0.3100 \times 10^{-4}$
 $cabs = 0.1 \times 10^3$, $e_r = 0.3333 \times 10^{-1}$

We note that the same relative error 0.3333×10^{-1} occurs for widely varying absolute errors.

As a measure of accuracy the absolute error can be misleading. The relative error is more meaningful since it takes into consideration the size of the value.

$$e_r = \frac{|x - x^R|}{|x|}$$

[This can be used to evaluate the percentage error = $(e_r \times 100)\%$]

1.5 Significant digits

Relative error (e_r) can be used to give a measure of significant digits of accuracy for an approximation.

Definition: The x^r is said to approximate to n significant digits (or figures) if n is the largest non-negative integer for which $\frac{|x - x^r|}{|x|} \leq 5 \times 10^{-n}$

Theorem:

If the first significant digit is an appropriate number x^r is k and the number is correct to n significant digits

$$e_r \leq \frac{1}{k10^{n-1}} \text{ or } \max e_r = \frac{1}{k10^{n-1}}$$

Proof:

Case 1:

Decimal point is assumed to the right most digit of the number x^r ie x^r is correct to 0 decimal places.

$$x^r = kd_2 d_3 \dots \dots \dots dn$$

$$cabs \leq .5 \times 10^{-0}$$

$$\leq .5$$

Substitute 0⁰s from all d_s in x^r

$$x^r \geq k 0 0 \dots \dots \dots .0$$

$$\geq k 10^{n-1}$$

We know that

$$e_r = \frac{cabs}{|x^r| - cabs}$$

$$e_r \leq \frac{.5}{|k10^{n-1}| - 0.5}$$

$$\leq \frac{1}{2k10^{n-1} - 1}$$

$$\text{Also } 2.k10^{n-1} - 1 = k.10^{n-1} - 1$$

$$(2.k10^{n-1} - 1) - k10^{n-1} = k.10^{n-1} - 1$$

$$2.k10^{n-1} - 1 > k.10^{n-1}$$

$$e_r \leq \frac{1}{k10^{n-1}}$$

$$\text{Max } e_r = \frac{1}{10^{n-1}}$$

Case 2:

Decimal point is placed anywhere i.e x^* is correct to m decimal places if x^* correct to n significant figures/digits

$$x^* = kd_2 d_3 \dots \dots \dots dp. \frac{dp+1d_{p+2} \dots \dots \dots dn}{m \text{ decimal places}}$$

$$= kd_2 d_3 \dots \dots \dots dp d_{p+1} d_{p+2} \dots \dots \dots dn$$

Corrected to 0 decimal places.

$$= k10^{n-1}$$

$$e_r \leq \frac{cabs}{|x| - cabs}$$

$$\text{Cabs in } x^* \leq .5 \times 10^{-m}$$

$$x^* = kx 10^{-m} \times 10^{-m}$$

$$e_r \leq \frac{.5 \times 10^{-m}}{k \times 10^{n-1} \cdot 10^{-m} - .5 \times 10^{-m}}$$

$$\leq \frac{1}{2k \cdot 10^{n-1} - 1} \leq \frac{1}{k \cdot 10^{n-1}}$$

$$\text{Max } e_r = \frac{1}{k \cdot 10^{n-1}}$$

Example:

$$936.73, \quad k = 9, \quad n = 5$$

$$\text{Max } e_r = \frac{1}{9 \times 10^{-4}} = \frac{1}{9} \times 10^{-4}$$

1.6 Propagation of errors in arithmetic operations

The error in the result of an arithmetic operation arising due to initial errors in the numbers used in that operation is called “the propagated error”. The total cumulative error at any step in the procedure is called “accumulated error”.

Let x and y be two exact numbers and let x^* and y^* be approximations with initial error ε (epsilon) and n (niu) respectively.

$$\text{i.e. } x = x^* + \varepsilon, \quad y = y^* + n$$

Let w be operation

$$x w y - x^* w^* y^* =$$

Exact no compute operation

w - Operation with errors

$$(x w y - x^* w y^*) + (x^* w y^* - x^* w^* y^*)$$

$$\begin{array}{ccc} \downarrow & & \downarrow \\ \text{Propagated error} & & \text{Generated error} \end{array}$$

Accumulated error = propagated error + generated error

Let the approximate numbers be x^*, y^* and exact numbers be x and y

$$x = x^* \pm \varepsilon$$

$$y = y^* \pm n$$

Addition and subtraction

$$(x \pm y) - (x^* \pm y^*) = e \text{ in } (x^* \pm y^*)$$

$$e = (x^* \pm \varepsilon) \pm (y^* \pm n) - ((x^* \pm y^*))$$

$$= (x^* + y^*) \pm (\varepsilon + n) - ((x^* \pm y^*))$$

$$e = \pm (\varepsilon \pm n)$$

$$|e| \leq |\varepsilon| + |n|$$

$$\max |e| = |\varepsilon| + |n|$$

Multiplication ($x^* \cdot y^*$)

$$e_{abs \text{ in } x^* y^*} = |xy - x^* y^*|$$

$$e_r \approx \frac{cabs}{|x^* y^*|}$$

$$\begin{aligned} cabs &= |(x^* \pm \varepsilon)(y^* \pm n) - x^* y^*| \\ &= |(x^* y^* \pm y^* x^* + \varepsilon y^* \pm \varepsilon n - x^* y^*)| \\ &= \pm n x^* x^* \pm \varepsilon y^* + \varepsilon n \end{aligned}$$

$$e_r = \left| \pm n x^* \pm \varepsilon y^* \pm \frac{\varepsilon n}{x^* y^*} \right|$$

$$e_r \approx \left| \frac{\varepsilon}{x^*} + \frac{n}{y^*} + \frac{\varepsilon n}{x^* y^*} \right|$$

$$e_r \leq \left| \frac{\varepsilon}{x^*} \right| + \left| \frac{n}{y^*} \right| + \left| \frac{\varepsilon n}{x^* y^*} \right|$$

Assuming that ε and n are so small the $\left| \frac{\varepsilon n}{x^* y^*} \right| \ll \left| \frac{\varepsilon}{x^*} \right|$ or $\left| \frac{n}{y^*} \right|$

$$e_r \leq \left| \frac{\varepsilon}{x^*} \right| + \left| \frac{n}{y^*} \right|$$

$$\text{Max } e_r = \left| \frac{\varepsilon}{x^*} \right| + \left| \frac{n}{y^*} \right| \text{ in } x^* y^*$$

Example 1

Suppose $x = \frac{5}{7}$, $y = \frac{1}{3}$ and that five digit chopping is used for arithmetic calculations involving x and y .

Floating point $fl(x) = 0.71428 \times 10^0$, $fl(y) = 0.33333 \times 10^0$

The table below shows the values for various operations.

Operation	Result	Actual value	Absolute error	Relative error
$x + y$	0.10476×10^1		0.190×10^{-4}	0.182×10^{-4}
$x - y$	0.38095×10^0		0.238×10^{-5}	0.625×10^{-5}
$x \times y$	0.23805×10^0		0.524×10^{-5}	0.220×10^{-4}
$x \div y$				

	0.21428×10^7		0.571×10^{-4}	0.267×10^{-4}
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Since the maximum relative error is 0.267×10^{-4} the arithmetic produces satisfactory five digit results.

Example 2:

If $u = 0.714251$, $v = 98765.9$, $w = 0.111111 \times 10^{-4}$

$$fl(u) = 0.71425 \times 10^0, \quad fl(v) = 0.98765 \times 10^5$$

$$fl(w) = 0.11111 \times 10^{-4}$$

The table below is used to demonstrate some problems that can arise with finite-digit arithmetic:

Operation	Result	Actual value	Absolute error	Relative error
$x + u$	0.30000×10^{-4}	0.3471×10^{-4}	0.471×10^{-5}	0.136
$(x - u) \div w$	0.27000×10^7	0.31243×10^7	0.424	0.136
$(x - u) \times v$	0.29629×10^7	0.34285×10^7	0.465	0.136
$u + v$	0.98765×10^5	0.98766×10^5	0.161×10^7	0.163×10^{-4}

The difference $x - u$ results in a small absolute error but a large relative error.

The subsequent division by the small number w or multiplication by a large number v magnifies the absolute error without modifying the relative error. The addition of the large and small numbers v and u produces large absolute error but not large relative error.

Example

- 1) Evaluate as accurately as possible $3.45 + 4.87$
 $3.45 + 4.87$
- 2) $x = 3.53 \pm 0.01$, $y = 2.73 \pm 0.02$ evaluate $x - y$ as accurately as possible.

- 3) $x = 3.55 + 0.005$, $y = 2.73 \pm 0.005$ find xy as accurately as possible.

Solutions

$$x^* = 3.45, \quad \varepsilon = 0.5 \times 10^{-2}$$

$$y^* = 4.87, \quad n = 0.5 \times 10^{-2}$$

Max e_r in $(x^* + y^*)$ is $|\varepsilon| + |n| = 0.01$

$$(x + y) \varepsilon (8.31, 8.33)$$

Rounding off to 1 d or 2sf

$$x - y = 8.3 \text{ correct to 1dp of 2sf}$$

Method 2

$$x = x^* \pm \varepsilon = 3.45 \pm 0.005$$

$$x \in (3.445, 3.455)$$

$$y = y^* \pm n = (4.87 \pm 0.005)$$

$$y \in (4.865, 4.875)$$

$$x + y \in (3.445 + 4.865, 3.455 + 4.875)$$

$$\varepsilon (8.31, 8.33) = 8.3$$

1.7 General formula for propagated error

Case 1: When a function f is a function of one variable $f(x)$: The error in $f(x)$ is represented by Δf

$$\Delta f = |f(x) - f(x^*)|$$

Using Taylor's series expansions around $x = x^*$

$$f(x) = f(x^*) + (x - x^*)f'(x^*) + \frac{(x - x^*)^2}{2!} f''(x^*) + \dots$$

If Δx is the error in x^* , that is $x = x^* \pm \Delta x$ or $x - x^* = \pm \Delta x$

$$\therefore f(x) - f(x^*) = \pm \Delta x f'(x^*) + \frac{(\Delta x)^2}{2!} f''(x^*) + \dots$$

$$f(x) - f(x^*) \approx \Delta x f'(x^*)$$

$$\text{or } \Delta f = |f'(x) - f(x^*)| \simeq |\Delta x f'(x^*)|$$

$$\text{Or } \Delta f \leq |f'(x^*)| \pm \Delta f$$

Case

$$f(x) = x^2 + 2x + 3$$

$$\text{Error in } f(2.5) = |f(2.55) - f(2.50)| = 0.2525$$

$$|f(2.5) - f(2.45)| = 0.2525$$

$$\Delta f = 0.05 (2 \times 2.5 - 2) = 0.05 (3) = 0.15$$

$$\therefore \Delta f = \sum_{i=1}^n [f(x_{i-1}) - f(x_i)]$$

$$\Delta f = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)_{x^*} \Delta x_i$$

$$|\Delta f| \leq \sum_{i=1}^n \left| \left(\frac{\partial f}{\partial x_i} \right)_{x^*} \right| |\Delta x_i|$$

If we represent $e_i = |\Delta x_i|$ we obtain

$$|\Delta f| \leq \sum_{i=1}^n \left| \left(\frac{\partial f}{\partial x_i} \right)_{x_i^*} \right| e_i \quad \text{ie the } f(x) \text{ make absolute error}$$

$$\sum_{i=1}^n \left| \left(\frac{\partial f}{\partial x_i} \right)_{x_i^*} \right| e_i$$

For example if $f(x, y) = xy$

$$e = \sum_{i=1}^n \left| \left(\frac{\partial f}{\partial x_i} \right)_{x_i^*} \right| e_i$$

where $x^* = x \pm \varepsilon$

$$x = x^* \pm \varepsilon, \quad y = y^* \pm n, \quad e_1 = \varepsilon, \quad e_2 = n$$

$$\begin{aligned}
 e &= \left(\frac{\partial f}{\partial x_i}\right) x^* y^* + \left(\frac{\partial f}{\partial x_i}\right) x^* y^* e_2 \\
 &= \left|\left(\frac{\partial f}{\partial x}\right) x^* y^*\right| e_i + \left|\left(\frac{\partial f}{\partial y}\right) x^* y^*\right| e_2 \\
 &= |y^*| \varepsilon + |x^*| n \\
 e_r \max(x^* y^*) &= \frac{|y^*| \varepsilon + |x^*| n}{|x^* y^*|} \\
 &= \frac{\varepsilon}{|x^*|} + \frac{n}{|y^*|}
 \end{aligned}$$



ACTIVITIES

Let $f(x_1 x_2 x_3) = x_1 x_2^2 / \sqrt{x_3}$ Determine the maximum error in evaluating f where $x_1 = 2.0 \pm 0.1$, $x_2 = 3.0 \pm 0.2$, $x_3 = 1.0 \pm 0.1$

Solution:

$$x^* = 2.0, \quad x_2^* = 3.0, \quad x_3^* = 1.0$$

$$e_1 = 0.1, \quad e_2 = 0.2, \quad e_3 = 0.1$$

$$e = \sum_{i=1}^3 \left| \left(\frac{\partial f}{\partial x_i}\right) x_1^* x_2^* x_3^* \right| e_i$$

$$\left(\frac{\partial f}{\partial x_1}\right) x_1^* x_2^* x_3^* = \frac{(x_2^*)^2}{\sqrt{x_3^*}} + \frac{3^2}{1^2} = 9.0$$

$$\left(\frac{\partial f}{\partial x_2}\right) x_1^* x_2^* x_3^* = \frac{2x_1^* x_2^*}{\sqrt{x_3^*}} = \frac{2 \cdot 2 \cdot 3}{1} = 12.0$$

$$\left(\frac{\partial f}{\partial x_3}\right) x_1^* x_2^* x_3^* = -1/2 \cdot \frac{x_1^* x_2^*}{(x_3^*)^{3/2}} = -1/2 \cdot 2 \cdot 9 = -9 = 9.0 \text{ absolute}$$

$$e = 9.0 \cdot 0.1 + 12.0 \cdot 0.2 + 9 \cdot 0.1 = 4.2$$

Hence

$$f(x) = f(x_1^* \ x_2^* \ x_3^*) \pm e \text{ since } f(x_1^* \ x_2^* \ x_3^*) = 18$$

$$= 18 \pm 4.2$$

$$f(x) \in (13.8 \quad 22.2)$$



SELF-TEST QUESTIONS

- 1) Compute the absolute error and relative error in approximation of p by p^*
 - (a) $p = \pi, \quad p^* = \frac{22}{7}$
 - (b) $p = \pi, \quad p^* = 3.1416$
 - (c) $p = e, \quad p^* = 2.718$
 - (d) $\sqrt{2}, \quad p^* = 1.414$
 - (e) $p = e^{10}, \quad p^* = 22000$
 - (f) $p = 10^n, \quad p^* = 1400$
 - (g) $p = 8, \quad p^* = 39900$

- 2) Perform the following computations
 - i) Exactly
 - ii) Using three digit chopping arithmetic
 - iii) Using thrice digit rounding arithmetic
 - iv) Compute the relative errors in (ii) and (iii)
 - (a) $\frac{4}{5} + \frac{1}{3}$
 - (b) $\frac{4}{5} \cdot \frac{1}{3}$
 - (c) $\left(\frac{1}{3} - \frac{3}{11}\right) + \frac{3}{20}$
 - (d) $\left(\frac{1}{3} + \frac{3}{11}\right) - \frac{3}{20}$

- 3) Use three-digit rounding arithmetic to perform the following calculations, compute the absolute error and relative error with the exact value determined to at least five digits.
 - (a) $133 - 0.499$
 - (b) $(121 - 0.327) - 119$
 - (c) $\frac{\frac{13}{14} - \frac{6}{7}}{2e^{-5.2}}$
 - (d) $-10\pi + 6e^{-3}/62$
 - (e) $\frac{\pi - \frac{22}{7}}{1/17}$



SELF-TEST QUESTIONS

- 4) Let $f(x) = e^x - e^{-x}$
- Find $\lim_{x \rightarrow 0} \left(\frac{e^x - e^{-x}}{x} \right)$
 - Use three digit rounding arithmetic to evaluate $f(0.1)$
 - Replace each exponential function with its third madawin polynomial, and repeat part (b)
 - The actual value is $f(0.1) = 2.003335000$. find the relative errors for the values obtained in parts (b) and (c) above.
- 5) Use four-digit rounding arithmetic (and example given earlier) to find most accurate approximations to the roots of the following quadratic equs compute the absolute errors and relative errors
- $\frac{1}{3}x^2 - \frac{123}{4}x + \frac{1}{6} = 0$
 - $\frac{1}{3}x^2 + \frac{123}{4}x - \frac{1}{6} = 0$
 - $1.002x^2 - 11.01x + 0.01265 = 0$
 - $1.002x^2 - 11.01x + 0.01265 = 0$
- 6) The two-linear system
- $$ax + by = e$$
- $$cx + dy = f$$
- Where a, b, c, d, e, f are given can be solved for x and y as follows:
- $$m = \frac{c}{a} \quad \text{provide } a \neq 0$$
- $$d_1 = d - mb$$
- $$f_1 = f - me$$
- $$y = \frac{f_1}{d_1}, \quad x = \frac{e - by}{a}$$
- Solve the following linear systems using four-digit rounding arithmetic
- $1.130x - 6.990y = 14.20 \quad x = 2.451$
 $1.0.13x - 6.990y = 14.20 \quad y = -1.635$
 - $8.110x + 12.20y = -0.1370 \quad x = 507.7$
 $-18.11x + 112.2y = -0.1376 \quad y = 82.0$
- 7) A rectangular parallel piped has sides 3cm, 4cm and 5cm measured to the nearest cm. what are the best upper and lower bounds for the
- Volume of the parallel piped
 - Surface area

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2. **Numerical Methods for Scientific and Engineering Computation: M. K. Jain**
3. **Numerical Analysis: Schaum's Outline Series**
4. **Advanced Engineering Mathematics: Arwin Kreyszig.**
4. **Any other relevant material (text) on Elementary Numerical Analysis.**

LECTURE TWO

POLYNOMIALS AND INTERPOLATION



2.1 INTRODUCTION

Collocation Polynomials can be expressed in a variety of alternative forms all equivalent but each suited to somewhat different circumstances. Approximation by polynomials is one of the oldest ideas in numerical analysis and still one of the most heavily used. In this chapter, we consider the problem of approximating a given function by a class of simple functions, mainly polynomials.



2.2 LECTURE OBJECTIVES

By the end of this lecture the learner should be able to:

- i) Define polynomial and express given polynomials in different forms.
- ii) Perform synthetic division on given polynomials to function values.
- iii) Derive collocation polynomials from given data.
- iv) Use interpolation and polynomials to find function values.

2.3 Zeros of polynomials and synthetic division

A polynomial of degree n has the form

$$P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0$$

Where a_i s called coefficients of P are constants and $a_n \neq 0$.

A number (ξ) is a solution of $f(x) = 0$ if $f(\xi) = 0$. Such a solution ξ is called a root or a zero of $f(x)$. Geometrically, the root of an equation is the value of x at which the graph of $y = f(x)$ intersects the x -axis. The value of $f(x)$ changes sign after the root. If $f(x)$ can be written as $f(x) = (x - \xi)^n g(x) = 0$ where $g(x) \neq 0$ then ξ is said to be a multiple root.

Any polynomial $P_n(x)$ may be expressed as

$$P(x) = (x - r)q(x) + R$$

where r is any number, $q(x)$ is a polynomial of degree $n - 1$ and R is a constant.

Synthetic division is an economical procedure (or algorithm) for producing the $q(x)$ and R of the division algorithm. It is often used to obtain R , which by the remainder theorem equals function value of r . Thus $P(r) = R$. If r is a root (solution) of $f(x) = 0$ then $R = 0$.

Procedure:

We will use the polynomial $x^2 + 5x + 6$

- i) First write the coefficients of the polynomial inside an upside - down division symbol leaving space after the coefficients.

$$\begin{array}{r|} & 1 & 5 & 6 \\ \hline \end{array}$$

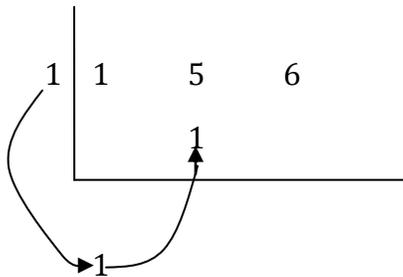
- ii) Put the test zero $x = 1$ at the left

$$\begin{array}{r|} 1 & 1 & 5 & 6 \\ \hline \end{array}$$

- iii) Take the first number inside, representing the leading coefficient and carry it down unchanged to become the division symbol

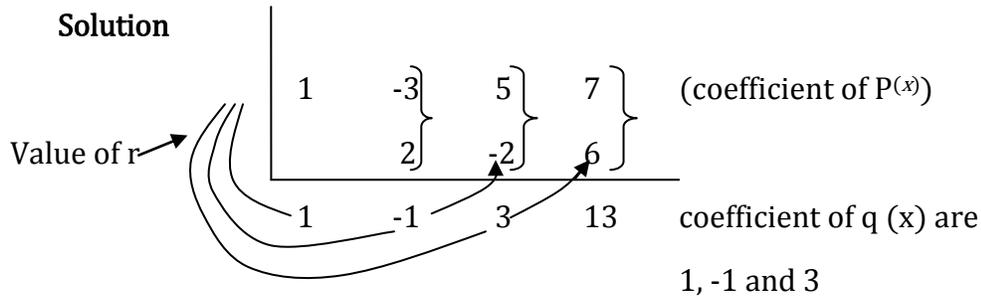
$$\begin{array}{r|} 1 & 1 & 5 & 6 \\ \hline & & & \\ \downarrow & & & \\ & 1 & & \end{array}$$

iv) Multiply this carry down value by the test zero and carry the result up into the next column.



Illustrate the “synthetic division” method for performing the division

i) Using $r = 2$ and $P(x) = x^3 - 3x^2 + 5x + 7$



$$q(x) = x^2 - x + 3$$

the remainder $R_s = 13$ and this is equal to

$$f(2) = 13$$

Therefore,

$$x^3 - 3x^2 + 5x + 17 = (x - 2)(x^2 - x + 3) + 13$$

ii) Using $r = 1$ and $P(x) = 2x^4 - 3x^2 + 3x - 4$

-2	2	0	-3	3	-4
	2	-4	0	-10	14
	2	-4	5	-7	10

$$P(-2) = 10 \quad q(x) = 2x^3 - 4x^2 + 5x - 7$$

Therefore

$$2x^4 - 3x^2 - 3x - 4 = (2x^3 - 4x^2 + 5x - 7)(x + 2) + 1$$

Exercise

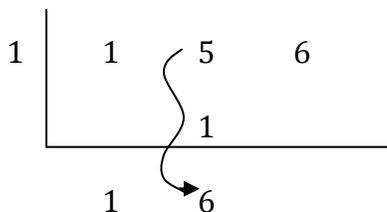
- Given $P(x) = 2x^4 - 24x^3 + 100x^2 - 168x + 93$
Use synthetic division to complete
 $P(1)$, $P(2)$, $P(-3)$
- Use synthetic division to evaluate $f(4)$ for each of the functions below

i) $x^5 - x^4 + 2x^3 - 3x^2 + x - 4$

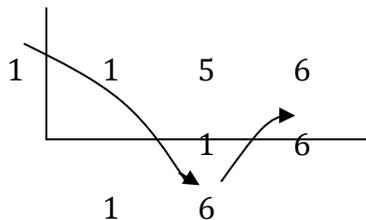
ii) $x^4 + 5x^3 - 9x^2 - 85x - 136$

- Use synthetic division to show that the polynomial equation $8x^3 - 12x^2 - 2x + 3 = 0$ has a root in the intervals $(-1, 0)$, $(0, 1)$, and $(1, 2)$.

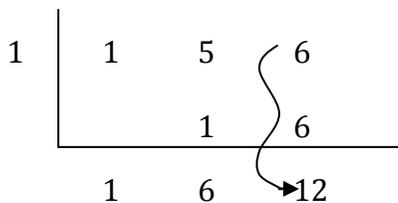
- Add down the column



- Multiply the previous carry down value by the test zero, and carry the new result up into the test column



- Add down the column



The numbers 1 and 6 are the coefficients of $q(x) = x + 6$ while the number 12 is the remainder which is $P(1)$ of $f(1)$

Therefore,



ACTIVITIES

Example 1

Show that the equation $x^3 - 2x^2 + 5 = 0$ has a root in the interval $(1, 4)$.

Solution

Here we find $f(1) = -6$ and $f(4) = 37$

$f(1)$ is negative while $f(4)$ is positive hence there is a root in $[1, 4]$.

2.4 Nested forms of polynomials

Mathematical expressions and polynomials can be written such that there are the fewest arithmetic operations.

For example

$x^3 - 6x^2 + 3x$ can be written as

$$x(x^2 - 6x + 3) = x[x(x - 6) + 3]$$

or $[(x - 6)x + 3]x$

This is called nested form and this reduces the relative error due to decreased number of computations.

To evaluate $f(x) = x^3 - 6x^2 + 3x - 0.14$ at $x = 4.17$

We substitute x into the nested form instead of the original polynomial.

$$f(4.17) = [(4.17 - 6)(4.17) + 3](4.17) - 0.149 = 14.5$$



SELF-TEST QUESTIONS

Use nested form of multiplication for $P(x) = 9x^5 - 20x^4 + 13x^3 + 7x^2 + 5x - 32$

2.3 Approximations by polynomials

Approximation by polynomials is commonly used in Numerical analysis. A polynomial $P(x)$ is used as a substitute for a function $y(x)$ and polynomials are easy to compute since only simple integer powers are used.

For example, Maclawins series

$$f(x) = e^x \approx 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots + \frac{x^n}{n!}$$

↑
 $p(x) =$

$$f(x) = \cos x \approx 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \dots + \frac{(-1)^k x^{2k}}{(2k)!}$$

↑
 $p(x) =$

The difference $f(x) - p(x)$ is the error of the approximation.

The collocation polynomial:

It coincides (collocates) with $y(x)$ at certain specified points. Given values of x_i and corresponding values of y_i , the collocation polynomial can be obtained.



ACTIVITIES

Find the first degree polynomial $P_1(x)$ which takes the values

$$y(0) = 1, y(1) = 0$$

Solution

This is linear since only two points are given

$$\frac{y-1}{x-0} = \frac{1-0}{0-1} \Rightarrow \frac{y-1}{x} = -1$$

$$y-1 = -x \Rightarrow y = 1-x$$

Therefore

$$P_1(x) = 1-x$$

Examples 2

To find a second degree polynomial which takes the following values.

$$x_i \quad 0 \quad 1 \quad 2$$

$$y_i \quad 0 \quad 1 \quad 0$$

Solution

$$\text{Let } p(x) = A + Bx + Cx^2$$

$$\text{Substituting } 0 = A$$

$$1 = A + B + C \Rightarrow B + C = 1$$

$$0 = A + 2B + 4C \Rightarrow 2B + 4C = 0$$

Solving

$$A = 0, B = +2 \text{ and } C = -1$$

Therefore

$$P(x) = 2x - x^2$$

The procedure above can be used for higher order $P_n(x)$ but is not very efficient since the number of equations to be solved increase as n increases

**SELF-TEST QUESTIONS****Exercise**

1. Find the unique cubic polynomial $P(x)$ which takes the following values

i)

x_i	0	1	2	3
y_i	0	1	16	8

ii)

x_i	4	6	8	10
y_i	1	3	8	20

2.6 Interpolation and polynomial approximations

A polynomial $P_n(x)$ is called an interpolating polynomial if the values of $P(x)$ and/or its certain order derivative coincide with those of x .

Theorem 1 (Weirstrauss approximation Theorem)

If $f(x)$ is defined in a continuous given interval (a, b) and $\epsilon > 0$, then there exists a polynomial $P(x)$ defined on $[a, b]$ with the properties.

If $||f(x) - P(x)|| < \epsilon$ such that $x \in (a, b)$.

In approximating we try to reduce the value of ϵ (error) as possible. In other words there exists a polynomial which approximates $f(x)$ uniformly to any required accuracy.

The Taylor polynomials are useful in determining approximations for certain functions but they are only accurate over small intervals. This is because all the information used in the approximation is concentrated at the single point x_0 , results become inaccurate as one moves away from x_0 .



ACTIVITIES

Find a polynomial $P_n(x)$ of degree 3 or less to approximate the function $f(x) = \sin x$, near $x_0 = 0$. And use this to approximate polynomial to approximate $\sin(0.1)$

Solution

We are required to find a polynomial which when substituted will be close to $\sin x$, small interval, close to a straight line.

Let $P_n(x) = a_0 + a_1x + a_2x^2 + a_3x^3$, we want to determine a_0, a_1, a_2, a_3 such that

$$P(0) = f(0), P'(0) = f'(0), P''(0) = f''(0) \text{ and } P'''(0) = f'''(0)$$

$$P(0) = a_0 = \sin 0 = 0$$

$$P'(x) = a_1 + 2a_2x + 3a_3x^2$$

$$P'(0) = a_1 = f'(0) = \frac{d}{dx}(\sin 0) = \cos 0 = 1$$

$$P''(x) = 2a_2 + 6a_3x$$

$$P''(0) = 2a_2 = f''(0) \sin 0 = 0$$

$$P'''(x) = 6a_3, P'''(0) = 6a_3 = -\cos 0 = -1$$

$$P_3(x) = x - \frac{1}{6}x^3$$

$$P(0.1) = 0.1 - \frac{1}{6}(0.1)^3 = 0.09983$$

$$\text{Exact value of } \sin(0.1) = 0.099833416$$

Accuracy increases with increase in n



SELF-TEST QUESTIONS

Exercise

- a) Determine the third degree Taylor polynomial about $x_0 = 0$ for $f(x) = \sqrt{1+x}$.
- b) Use the polynomial in part (a) to
 - i) Approximate $\sqrt{1.1}$ and find a bound for the error involved.
 - ii) To approximate $\int_0^{0.1} \sqrt{1+x} dx$ and find a bound for the error of this approximation.

2.5 Interpolations and the Lagrange polynomial

Theorem 2 therefore if $x_0, x_1, x_2, \dots, x_n$ are in $(n + 1)$ distinct numbers and f is a function whose values are given at these numbers then there exists a unique polynomial $p(x)$ of degree at most n with the property.

$$f(x_k) = P(x_k) \text{ for each } k = 0, 1, \dots, n$$

The polynomial is given by

$$P(x) = f(x_0) L_{n,0}(x) + f(x_1) L_{n,1}(x) + \dots + f(x_n) L_{n,n}(x) \\ = \sum_{k=0}^n f(x_k) L_{n,k}(x) \dots \dots \dots (1)$$

$$\text{Where } L_{n,k}(x) = \frac{n!}{(n-k)!k!} \frac{(x-x_0) \dots (x-x_{k-1})(x-x_{k+1}) \dots (x-x_n)}{(x_k-x_0) \dots (x_k-x_{k-1})(x_k-x_{k+1}) \dots (x_k-x_n)} \dots \dots \dots (2)$$

$$i = 0$$

$$i \neq k$$

$$L_{n,k}(x) = \frac{(x-x_0) \dots (x-x_{k-1}) \dots (x-x_{k+1}) \dots (x-x_n)}{(x_k-x_0) \dots (x_k-x_{k-1}) \dots (x_k-x_{k+1}) \dots (x_k-x_n)}$$

(Avoid $(x - x_k)$ in the numerator and $(x_k - x_k)$ in the denominators).

The above polynomial is called the n^{th} Lagrange interpolating polynomial.

To obtain it we:

- i) Determine Lagrange fundamental polynomials
- ii) Multiply by the corresponding function values
- iii) Add them together.



ACTIVITIES

Write out the Lagrange fundamental polynomials (cardinal functions) appropriate to the problem of interpolating the table below. Hence find the Lagrange interpolating polynomial

x	$\frac{1}{3}$	$\frac{1}{4}$	1
$f(x)$	2	-1	7

Solution

$$L_0(x) = \frac{(x - \frac{1}{4})(x - 1)}{(\frac{1}{3} - \frac{1}{4})(\frac{1}{3} - 1)} = -18(x - \frac{1}{4})(x - 1)$$

$$L_1(x) = \frac{(x - \frac{1}{3})(x - 1)}{(\frac{1}{4} - \frac{1}{3})(\frac{1}{4} - 1)} = 16(x - \frac{1}{3})(x - 1)$$

$$L_2(x) = \frac{(x - \frac{1}{3})(x - \frac{1}{4})}{(1 - \frac{1}{3})(1 - \frac{1}{4})} = 2(x - \frac{1}{3})(x - \frac{1}{4})$$

The polynomial of degree 2 is

$$\begin{aligned} P^2(x) &= L_0(x) + (-1)L_1(x) + (7)L_2(x) \\ &= [2(-18)(x - 1)(x - \frac{1}{4}) + x - \frac{1}{3}] + 7(2)(x - \frac{1}{3})(x - \frac{1}{4}) \end{aligned}$$

$$P^2(x) = 2 + (x - \frac{1}{3})[36 + (x - \frac{1}{4})(-38)]$$

This polynomial is accurate in the vicinity of the nodes $\frac{1}{3}$, $\frac{1}{4}$ and 1-



SELF-TEST QUESTIONS

1. Determine the 2nd degree interpolating polynomial for the function $f(x) = \frac{1}{x}$ using the nodes $x_0 = 2$, $x_1 = 2.5$ and $x_2 = 4$
2. Find the polynomial of degree three which takes the values prescribed below.

x_k	0	1	2	4
y_k	1	1	2	5

3. Use Lagrange's formula to produce a cubic polynomial which collocates the following (x_k, y_k) number pairs.
Hence evaluate this polynomial values (interpolate) for $x = 2$ and 3

x_k	0	1	4	6
y_k	1	-1	1	-1

4. Use the Lagrange interpolation process to obtain a polynomial of at least degree three that assumes the values below.

x	0	2	3	4
y	7	11	28	63

**REFERENCES**

1. **Numerical Analysis: Richard L. Burden, J. Douglas Faires**
2. **Numerical Methods for Scientific and Engineering Computation: M. K. Jain**
3. **Numerical Analysis: Schaum's Outline Series**
4. **Advanced Engineering Mathematics: Arwin Kreyszig.**
4. **Any other relevant material (text) on Elementary Numerical Analysis.**

LECTURE THREE

FINITE DIFFERENCES



3.1 INTRODUCTION

Given values of $f(x)$ at specific points x_n approximate value of $f(x)$ for any x within the interval can be obtained using an appropriate polynomial. This process is interpolation. In this lecture various interpolation techniques involving finite differences for discrete data are discussed.



3.2 LECTURE OBJECTIVES

By the end of this lecture the learner should be able to:

- i) Define the terms forward, central and backward differences.
- ii) Construct finite difference tables.
- iii) Detect and correct errors in given data by using finite differences.
- iv) Use Newton's Forward or Backward difference to construct polynomials from equally spaced points.
- v) Use the method of Newton's Divided Difference for unequally spaced points.

3.3. Finite difference table

Finite difference are very useful to mathematics and have been in use since the days of Isaac Newton. Given a discrete function that is a finite set of arguments x_i , each having a mate y_i and supposing the arguments are equally spaced so that $x_{i+1} - x_i = h$ the differences of the y_i values are denoted by

$$\Delta y_i = y_{i+1} - y_i$$

and are called the first differences.

The differences of these first differences are denoted by

$$\begin{aligned} \Delta^2 y_i &= \Delta(\Delta y_i) = \Delta y_{i+1} - \Delta y_i \\ &= y_{i+2} - 2y_{i+1} + y_i \end{aligned}$$

and are called second differences

In general $\Delta^n y_i = \Delta^{n-1} y_{i+1} - \Delta^{n-1} y_i$ defines the n^{th} differences

The differences table is the standard format for displaying finite differences its diagonal pattern makes each entry expect for x_i, y_i , the difference of its two nearest neighbours to the left given a table

x_i	x_0	x_1	x_2	x_3	x_4
y_i	y_0	y_1	y_2	y_3	y_4

The corresponding difference table would be

x_i	y_i	1st order Δy_i	2nd order $\Delta^2 y_i$	3rd order $\Delta^3 y_i$	4th order $\Delta^4 y_i$
x_0	y_0				
x_1	y_1	Δy_0			
x_2	y_2	Δy_1	$\Delta^2 y_0$		
x_3	y_3	Δy_2	$\Delta^2 y_1$	$\Delta^3 y_0$	
x_4	y_4	Δy_3	$\Delta^2 y_2$	$\Delta^3 y_1$	$\Delta^4 y_0$

Each difference proves to be a combination of the y values in column two.

For example

$$\Delta^3 y_0 = \Delta^2 y_1 - \Delta^2 y_0$$

$$(y_3 - 2y_2 + y_1) - (y_2 - 2y_1 + y_0)$$

$$y_3 - 3y_2 + 3y_1 - y_0$$

For any positive integer I

$$\Delta^i y_0 = \sum_{r=0}^i (-1)^r \binom{i}{r} y_{i-r}$$

$$\text{where } \binom{i}{r} = \frac{i!}{r!(i-r)!}$$

Example

Let f be a function of x or $y = f(x)$ with corresponding values as given below

x	1	2	3	4	5	6
$f(x)$	-4	-2	2	14	40	86

$$x_i = x_0, x_1 \text{ ----- } x_5$$

$$y_i = y_0, y_1 \text{ ----- } y_5$$

To construct

The corresponding difference table we start by listing the values of x_i and y_i leaving a line between x_i and x_{i+1} , then proceed to calculate the differences

x_i	y_i	1st order Δy_i	2nd order $\Delta^2 y_i$	3rd order $\Delta^3 y_i$	4th order $\Delta^4 y_i$
1	4				
2	-2	$(-2 - 4) = 2$			
3	2	$(2 - (-2)) = 4$	$(4 - 2) = 2$		
4	14	$(14 - 2) = 12$	$(12 - 4) = 8$	$(8 - 2) = 6$	0
5	40	$(40 - 14) = 26$	$(26 - 12) = 14$	$(14 - 8) = 6$	0
6	86	$(86 - 40) = 46$	$(46 - 26) = 20$	$(20 - 14) = 6$	

Which takes the form?

x_i	y_i	1st order Δy_0	2nd order $\Delta^2 y_0$	3rd order $\Delta^3 y_0$	4th order $\Delta^4 y_0$
1	4				
2	-2	2			
3	2	4	2		
4	14	12	8	6	0
5	40	26	14	6	0
6	86	46	20	6	0



ACTIVITIES

Construct a difference table for $f(x) = e^x$ for $x \in \left[\frac{0}{10}, 0.16\right]$ with $h = 0.01$

Solution:

The given function and interval are used to construct data points for (x_i, y_i)

i	x_i	y_i	Δy_0	$\Delta^2 y_0$	$\Delta^3 y_0$
0	0.10	1.10517			
			0.01111		
1	0.11	1.11628		0.000111	
			0.01122		0
2	0.12	1.12750		0.00011	0
			0.01133		0
3	0.13	1.13883		0.00011	0
			0.01144		0
4	0.14	1.15027		0.00011	0
			0.01155		0
5	0.15	1.16183		0.00011	
			0.01166		
6	0.16	1.17351			

- If the function is well behaved (thus) continuously decreasing or increasing) the higher order differences decrease in magnitude rapidly.
- If there are n tabular points we could obtain the differences upto $(n - 1)$ th order.
- If round off errors are negligible in functional values higher order differences are constants or nearly constants and $\Delta C = 0$



SELF-TEST QUESTIONS

1. Prove that $\Delta^4 y_4 = y_4 - 4y_3 + 6y_2 - 4y_1 + y_0$
2. Compute through third differences of the discrete function in the table below

i	0	1	2	3	4	5	6	7
x_i	1	2	3	4	5	6	7	8
y_i	1	8	27	64	125	216	343	512

3. Construct a difference table for the data below

x_i	0	1	2	3	4	5	6
y_i	0	1	16	81	256	625	1296

3.4 Detection and correction of errors

Let there be an error e in one of the tabulated functional values. The difference table will be as follows:

<i>Error</i>	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
0	0					
0	0	0				
0	0		e			
0	e	e		$-4e$		
e	e	$-2e$	$-3e$		$10e$	
	$-e$	$-2e$	$3e$	$6e$		$-20e$
0		e	$3e$	$-10e$		
0	0		$-e$	$-4e$		
0		0				
0	0					

- i) It is noted that the error spreads and has a larger magnitude for every successive difference

- ii) The coefficient error e in the n^{th} order differences are the same as the binomial coefficients of $(1-x)^n$ for example coefficients of Δ^3 are $1, 3, 3, -1$ since $(1-x)^3 = 1 - 3x + 3x^2 - x^3$



ACTIVITIES

Detect and correct one error in the data below

x	0	1	2	3	4	5	6	7	8	9	10
$f(x)$	3	2	3	6	11	18	21	38	51	66	83

Solution

Constructing a difference table

x	$f(x)$	Δ	Δ^2	Δ^3
0	3			
		-1		
1	2		2	
		1		0
2	3		2	
		3		0
3	6		2	
		5		0
4	11		2	
		7		-6
5	18		-4	
		3		18
6	21		14	
		17		-18
7	38		-4	
		13		6
8	51		2	
		15		0
9	66		2	
		17		
10	83			

Third order differences (Δ^3) have errors in the ratio $(-6,18,-18,6)$ which correspond to the binomial coefficients for $(1-x)^3$, thus $(1,-3,3,-1)$ multiplied by the error

$$e, -3e, 3e, -e = (-6,18,-18,6)$$

$$\therefore e = -6$$

The error is in the value $f(6) = 21$

The actual value = $21 - (-6) = 27$



ACTIVITIES

Example 2

Find and correct a misprint in the data below:

y_i	1	11	31	69	113	223	357	521	739	1911
-------	---	----	----	----	-----	-----	-----	-----	-----	------

Solution

Difference table

y_i	Δ	Δ^2	Δ^3	Δ^4
1				
→ 2				
3		→ 6		
→ 8		→ 6		
11	→ 12		→ 0	
→ 20	→ 6			
31	→ 18		→ 18	
→ 38	→ -12			
69	→ 6		→ 72	
→ 44		→ 60		
113	→			
		→ 66		→ 108
223	→ 110	→ -48		
→	→ 18		→ 122	
351	→ 128	→ 24		
		→ 42	→ -18	

$$\begin{array}{ccccccc}
 521 & \rightarrow & 170 & \rightarrow & & & \\
 & & & \rightarrow & 48 & \rightarrow & 6 \\
 739 & \rightarrow & 218 & \rightarrow & & \rightarrow & 0 \\
 & \rightarrow & & \rightarrow & 54 & \rightarrow & 6 \\
 1011 & & 272 & & & &
 \end{array}$$

The fourth differences $(-18, 72, -108, 72, -18) \equiv (1, -4, 6, -4, 1)$

The error $e = -18$

The error is in $y_i = 113$

$\therefore 131$ was misprinted as 113



SELF-TEST QUESTIONS

1. Find and correct a single error in these values

i	0	1	2	3	4	5	6	7
y_i	0	0	1	6	24	60	120	210

2. Find and correct a misprint in the list below

1 2 4 8 16 26 42 64 93

3. The table below has one incorrect entry for $f(x)$. Locate and correct the wrong value

x	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
$f(x)$	1.000	1.029	1.060	1.099	1.152	1.225	1.342	1.455	1.624	1.837	2.100

3.5 Notations for Finite difference

There are three notations for the finite difference

- Forward difference Δ
- Backward difference ∇
- Central differences δ

The shift operator is denoted by E.

- The shift operator E: this means shifting of one functional value to another. Let f_i be the functional value at x_i such that $f(x_0) = f_0, f(x_1) = f_1, \dots, f(x_n) = f_n$

The shift operator is defined as

$$E f_i = f_{i+1} \quad \text{or } f_i \rightarrow E \rightarrow f_{i+1}$$

- The forward difference operator Δ :

This is defined as $\Delta = E - 1$

The first difference is

$$\Delta f_i = (E - 1)f_i = E f_i - f_i = f_{i+1} - f_i$$

the second difference is

$$\Delta^2 f_i = (E - 1)^2 f_i = (E^2 - 2E + 1)f_i$$

$$\Delta^k f_i = (E - 1)^k f_i$$

- The backward difference operator ∇

This is defined as

$$\nabla f_i = f_i - f_{i-1} = (1 - E^{-1})f_i = \left(1 - \frac{1}{E}\right) f_i$$

$$\nabla^2 f_i = (1 - E^{-1})^2 f_i = (1 - 2E^{-1} + E^{-2})f_i$$

$$= f_i - 2f_{i-1} + f_{i-2}$$

$$\nabla^k f_i = (1 - E^{-1})^k f_i$$

- Central difference operator δ

This is defined as

$$\delta = E^{1/2} - E^{-1/2}$$

the first central difference at x_i is

$$\delta^2 f_i = (E^{1/2} - E^{-1/2})f_i = E^{1/2}f_i - E^{-1/2}f_i$$

$$\delta^2 f_i = (E^{1/2} - E^{-1/2})^2 f_i = (E - 2 + E^{-1}) f_i$$

- Relations between Δ, δ and ∇

All the three are defined in terms of the famous operator ∇ and hence they are related

$$\Delta = E - 1 = E(1 - E^{-1}) = E\nabla$$

$$= E^{1/2}(E^{1/2} - E^{-1/2}) = E^{1/2}\delta$$

3.6 Newton’s forward difference formula

This applies to equally spaced x_i s thus $x_0, x_1 = x_0 + h, x_2 = x_0 + 2h - - - -$ with corresponding y_i s

The collocation polynomial can be expressed in terms of finite differences and factorial polynomials. The summation formula

$$y_k = \sum_{i=0}^k \binom{k}{i} \Delta^i y_0$$

leads directly to Newton formula for collocation polynomial written as

$$P_k = \sum_{i=0}^k \binom{k}{i} \Delta^i y_0$$

an alternative form of the formula in terms of the argument x_k may be obtained using $x_k = x_0 + kh$ and proves to be

$$P(x_k) = y_0 + \frac{1}{h} (\Delta y_0) (x_k - x_0) + \left(\frac{\Delta^2 y_0}{2! h^2} \right) (x_k - x_0)(x_k - x_1) + - - - -$$

$$\left(\frac{\Delta^3 y_0}{3! h^3} \right) (x_k - x_0)(x_k - x_1)(x_k - x_2) + - - - - -$$

$$\left(\frac{\Delta^n y_0}{n! h^n} \right) (x_k - x_0)(x_k - x_1) - - - - (x_k - x_{n-1})$$

where $\Delta y_0, \Delta^2 y_0 - - - \Delta^n y_0$ are forward following differences



ACTIVITIES

Find the polynomial of degree three which takes the four values listed in the table below

x_k	4	6	8	10
y_k	1	3	8	20

Solution

We first construct a difference table

K	x_k	y_k	Δy_k	$\Delta^2 y_k$	$\Delta^3 y_k$
0	4	1			
1	6	3	2		
2	8	8	5	3	
			12	7	4

3 10 20
 $\Delta^n y_0$ values have been circled. The values are upto $\Delta^3 y_0$ which shows the polynomial is of degree three

$$P(x_k) = 1 + \frac{2(x-)}{1!2} + \frac{3(x-4)}{2!4} (x-6) + \frac{4(x-4)(x-6)(x-8)}{3!8}$$

$$= 1 + (x-4) + 3 \frac{(x^2 - 10x + 24)}{16} + \frac{(x-8)(x^2 - 10x + 24)}{12}$$



ACTIVITIES

Apply Newton’s formula to find a polynomial of degree four or less which takes the values

3.7 Divided differences

The collocation polynomial for unequally spaced arguments x_0, x_1, \dots, x_n may be found using lagrange polynomials and divided differences.

Let the data be of the

x_i	x_i	x_2	-----	$3x_n$
f_i	$f(x_1)$	$f(x_2)$	-----	$f(x_n)$

A divided difference table takes the form below

x_i	$f[x_1]$	$f[-,-]$	$f[-,-,-]$	$f[-,-,-,-]$
x_1	$f[x_1]$			
x_2	$f[x_2]$	$f[x_2, x_3]$	$f[x_1, x_2, x_3]$	$f[x_1, x_2, x_3, x_4]$
x_3	$f[x_3]$	$f[x_2, x_3]$	$f[x_2, x_3, x_4]$	
x_4	$f[x_4]$	$f[x_3, x_4]$		

The formula flowing diagonal coefficients are the ones needed to form the Newton’s interpolating polynomial. These values are calculated as follows:

$$f[x_i] = f(x_i)$$

$$f[x_i, x_2] = f\left(\frac{f(x_2) - f(x_i)}{x_2 - x_i}\right), \quad f[x_2, x_3] = f\left(\frac{f(x_3) - f(x_2)}{x_3 - x_2}\right)$$

$$f[x_i, x_2, x_3, x_4] = f\left(\frac{[f(x_2, x_3, x_4)] - [f(x_2, x_3, x_4)]}{x_4 - x_i}\right)$$

The resulting Newton's divided difference formula is

$$p_n(x) = f_0(x) + (x - x_0)f[x_0, x_1] + (x - x_0)(x - x_1)f[x_0, x_1, x_2]$$

Example $+ \dots + (x - x_0)(x - x_1) \dots (x - x_{n-1})f[x_0, \dots, x_n]$

Compute divided differences through the third for the $f(x_i)$ values below.

Hence find the collocation polynomial.

x_i	0	1	2	4
$f(x_i)$	1	1	2	5

Solution:

$$f[0, 1] = \frac{1-1}{1-0} = 0, \quad f[1, 2] = \frac{2-1}{2-1} = 1$$

$$f[2, 4] = \frac{5-2}{4-2} = 3/2,$$

$$f[0, 1, 2] = \frac{1-0}{2-0} = 1/2, \quad f[1, 2, 4] = \frac{3}{4-1} - 1 = 1/6$$

$$f[0, 1, 2, 4] = \left(\frac{1/6 - 1/2}{4-0}\right) = -1/12,$$

The divided difference table can be displayed as

x_i	$f(x_i)$	$f[-, -]$	$f[-, -, -]$	$f[-, -, -, -]$
0	1			
1	1	0		
2	2	$3/2$	$1/6$	
3	5			$-1/12$

The polynomial is given by taking the circled coefficients admit is of degree 3.

$$p_3(x) = 1 + 0(x - 0) + \frac{1}{2}(x)(x - 1) - \frac{1}{12}(x)(x - 1)(x - 2)$$

$$= \frac{1}{12}(-x^3 + 9x^2 - 8x + 12)$$

Example 2

Find the collocation polynomial for the data in the table below. Hence find $f(3)$

x_i	1	2	4	6
$f(x_i)$	1	8	6.4	216

Solution

The data is unequally spaced and so we construct a divided difference table.

x_i	$f(x_i)$	$f[-,-]$	$f[-,-]$	$f[-,-,-,-]$
1	1			
2	8	7		
		28		
4	6.3		7	1
			12	
6	216			

The divided difference polynomial is of order three.

$$\begin{aligned}
 p_3(x) &= 1 + 7(x-1) + 7(x-1)(x-2) + 1(x-1)(x-2)(x-4) \\
 &= 1 + 7x - 7 + 7x^2 - 2(x+14) \\
 &= x^3 - 6x^2 + 8x - x^2 - 6x - 8 \\
 &= p_3(x) = x^3 \\
 f(3) &= 3^3 = 27
 \end{aligned}$$

Exercise

- 1) Construct divided difference for the data below and determine the collocation polynomial

x_i	0	1	2	4	5
-------	---	---	---	---	---

(a)

$f(x_i)$	0	16	48	88	0
----------	---	----	----	----	---

(b)

x_i	0	1	4	6
$f(x_i)$	-0	-1	1	-1

(c)

x_i	1	$\frac{3}{2}$	0	2
$f(x_i)$	3	$\frac{13}{4}$	3	$\frac{5}{3}$

2) Consider the value of x_i and $f(x_i)$ given in the table below.

x	-1	0	2	3	4
$f(x)$	2	1	5	10	17

- (i) Construct a divided difference table for the above data and use it to determine the divided difference interpolating polynomial.
- (ii) Using the Lagrange interpolating formula determine the collocation polynomial for the data.
- (iii) Using the polynomials in (i) and (ii) compute $f(i)$ and compare the results.



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1. **Numerical Analysis: Richard L. Burden, J. Douglas Faires**
2. **Numerical Methods for Scientific and Engineering Computation: M. K. Jain**
3. **Numerical Analysis: Schaum's Outline Series**
4. **Advanced Engineering Mathematics: Arwin Kreyszig.**
4. **Any other relevant material (text) on Elementary Numerical Analysis.**

LECTURE FOUR

NUMERICAL DIFFERENTIATION



4.1 INTRODUCTION

Several methods are available to find the derivative of a function $f(x)$. However, when $f(x)$ is a complicated function or when given in a tabular form, we use numerical methods.



4.2 LECTURE OBJECTIVES

By the end of this lecture the learner should be able to:

- i) Obtain first and second derivatives using methods based on interpolation.
- ii) Obtain derivatives using finite differences.
- iii) Determine derivatives at non-tabular points.
- iv) Compute errors involved in numerical differentiation.

4.3 Definition of derivative

The first derivative of a function $f(x)$ is given by

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

Approximate derivatives of a function $f(x)$ may be found from a polynomial approximation $P(x)$ simply by accepting p' , $p^{(2)}$, $p^{(3)}$ ----- in place of f' , $f^{(2)}$, $f^{(3)}$ -----.
Collocation polynomials lead to variety of formulae such as:

$$i) \quad f'(x) \simeq \frac{f(x+h) - f(x)}{h}$$

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

$$iii) \quad f'(x) \simeq \frac{f(x) - f(x-h)}{h}$$

In each case only one term is being used and errors are expected. The accuracy of derivatives tends to diminish with increasing order of the derivatives. For example $f(x) - p(x)$ may be very small while $f'(x) - p'(x)$ is very large. Geometrically two curves may be close together but still have different slopes. The reciprocal power of h in the derivatives also magnify the error.

Numerical differentiation methods are obtained using methods based on interpolation, finite difference operators and undertrained coefficients.

4.4 Methods based on interpolation

This involves :

- (i) Obtaining the polynomial $P_n(x)$ and differentiating $P_n(x)$ r times to get the r^{th} derivative $P_n^{(r)}(x)$. The approximation error at any point x is given by

$$E^r(x) = f^{(r)}(x) - P_n^{(r)}(x)$$

- (ii) Using tabular points and Lagrange formula

$$P(x) = l_0 f_0 + l_1 f_1 + \dots + \dots + l_n f_n$$

$$P'(x) = l'_0 f_0 + l'_1 f_1 + \dots + \dots + l'_n f_n$$



ACTIVITIES

Given the following values of $f(x) = \log x$, find the approximate value of $f'(2.0)$ and $f''(2.0)$ using the methods based on linear and quadratic interpolation

x_i	2.0	2.2	2.6
f_i	0.69315	0.78846	0.95551

Solution

- i) Linear interpolation:
Consider the line joining (x_0, f_0) and (x_1, f_1)

$$f'(x_0) = \frac{f_1 - f_0}{x_1 - x_0} = \frac{0.78846 - 0.69315}{2.2 - 2.0} = 0.47655$$

- ii) Quadratic interpolation
This is derived from Lagrange formula for unequally spaced nodes
 $p_2(x) = l_0(x)f_0 + l_1(x)f_1 + l_2(x)f_2$

$$\frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f_2$$

Differentiating

$$P_2'(x) = \frac{(2x_0 - x_1 - x_2)}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{(x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{+(x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} f_2$$

$$f'(x_0) \simeq P_2'(x_0)$$

$$f'(2.0) = \frac{4 - 2.2 - 2.6}{(2.2 - 2.2)(2.2 - 2.6)} (0.69315) + \frac{2 - 2.6}{(2.2 - 2)(2.2 - 2.6)} (0.78846) + \frac{2 - 2.2}{(2.6 - 2)(2.6 - 2.2)} (0.95551) = 0.49619$$

The exact value of $f'(x)$ is given by

$$f(x) = \ln x, \quad f'(x) = \frac{1}{x}, \quad f'(2) = 0.5$$

Hence the quadratic interpolation is more accurate than linear

Similarly

$$f'' x_0 = \frac{2 f_0}{(x_0-x_1)(x_0-x_1)} + \frac{f_1}{(x_1-x_0)(x_1-x_2)} + \frac{f_2}{(x_2-x_0)(x_2-x_1)}$$

Which is constant for all $x \in [x_0, x_2]$

$$f'' (2.0) = \frac{0.69315}{(-0.2)(-0.6)} + \frac{0.78846}{(0.2)(-0.4)} + \frac{0.95551}{(0.6)(0.4)}$$

$$\text{Exact value } f''(x) = -1/x^2, \quad f''(2) = -0.25$$

The error in the second derivative is greater than error in the first derivative.

4.5 Methods based on finite differences

We consider the relation

$$\begin{aligned} Ef(x) = f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \dots \\ &= \left(1 + hD + \frac{h^2 D^2}{2!} + \dots \dots \dots\right) f(x) = e^{hD} f(x) \end{aligned}$$

in which $D = \frac{d}{dx}$ is called the differential operator symbolically we get $e^{hD} = E$

$$hD = \log E$$

$$D = \frac{1}{h} \log E = \frac{1}{h} \log(1 + \Delta) \text{ since } E = (1 + \Delta)$$

i) Using forward difference

$$D = \frac{1}{h} \log(1 + \Delta)$$

$$\begin{aligned} f'(x) = \Delta f_i &= \frac{1}{h} \log(1 + \Delta) f_i = \frac{1}{h} \left[\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots \dots \right] f_i \\ &= \frac{1}{h} \left[\Delta - \frac{1}{2} \Delta^2 f_i + \frac{1}{3} \Delta^3 f_i - \dots \dots \right] \end{aligned}$$

Then the second derivative

$$\begin{aligned} f''(x) &= \Delta^2 f_i = \Delta (\Delta f_i) = \frac{1}{h^2} (\ln E \ln E) f_i = \frac{1}{h^2} \ln(1 + \Delta) \ln(1 + \Delta) f_i \\ &= \frac{1}{h^2} \left[\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} + \frac{\Delta^4}{4} \dots \dots \dots \right] \left[\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} \dots \dots \dots \right] f_i \\ &= \frac{1}{h^2} \left[\Delta^2 - \Delta^3 + \frac{11}{12} \Delta^4 - \frac{5}{6} \Delta^5 + \dots \right] f_i \end{aligned}$$

Truncating at the first term

$$f'(x) \simeq \frac{\Delta}{h} f_i \quad \text{with error } E = \frac{-\Delta^2}{2h} f(\varepsilon)$$

and $f''(x) \simeq \frac{\Delta^2}{2} f_i \quad \text{with } E' = \frac{\Delta^3}{h^2} f(\varepsilon)$

So that

$$\Delta^2 f(\varepsilon) \simeq h^2 f''(\varepsilon) \quad \text{where } x_i < \varepsilon < x_h$$

$$E = -\frac{1}{2h} h^2 f''(\varepsilon) \quad \text{and } E' = h f''(\varepsilon)$$

ii) Using the backward difference

$$\Delta = \frac{1}{h} \ln E, \quad \text{where } E = (1 - \nabla)^{-1}$$

$$= \frac{1}{h} \ln(1 - \nabla)^{-1} = -1/h \ln(1 - \nabla) = \left[\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \dots \right] f_i$$

$$= -1/h \left[\nabla f_i + \frac{\nabla^2}{2} f_i + \frac{\nabla^3}{3} f_i + \frac{\nabla^4}{4} f_i + \dots \dots \right]$$

Second derivative

$$f''(f_i) = \Delta^2 f_i$$

$$= \frac{1}{h^2} [\ln(1 - \nabla)^{-1} \ln(1 - \nabla)^{-1}] f_i$$

$$= \frac{1}{h^2} [\ln(1 - \nabla) \ln(1 - \nabla)] f_i$$

$$= \frac{1}{h^2} \left[\nabla^2 + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \dots \right] \left[\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \dots \right]$$

$$= \frac{1}{h^2} \left[\nabla^2 + \nabla^3 + \frac{11}{12} \nabla^4 + \frac{5}{6} \nabla^5 + \dots \right] f_i$$

$$f''(x_i) = \frac{1}{h^2} \left(\nabla^2 f_i + \nabla^3 f_i + \frac{11}{12} \nabla^2 f_i + \frac{5}{6} \nabla^5 f_i + \dots \right)$$

Truncating at the first term

$$f''(x_i) \approx \frac{1}{h} \nabla f_i \quad \text{with } E \approx \frac{h}{2} f''(\varepsilon)$$

$$f''(x_i) \approx \frac{1}{h^2} \nabla^2 f_i \quad \text{with } E' = h f''(\varepsilon)$$

Where $x_i < \varepsilon < x_h$

4.6 Derivatives at tabular points

Let the non-tabular points be $x = x_i + sh$ Newton's interpolating polynomial using forward differences

$$f(x) = f(x_i + sh) = P_n(s)$$

$$= f_i + s \Delta f_i + \frac{s(s-1)}{2!} \Delta^2 f_i + s(s-1)(s-2) \frac{\Delta^3}{3!} f_i + \dots$$

$$f'(x) = \frac{d}{ds} (P_n(s)) = \frac{d}{ds} P_n(s) \frac{ds}{dx}$$

$$\text{from } x = x_i + sh \Rightarrow \frac{ds}{dx} = \frac{1}{h}$$

$$f'(x) = \frac{1}{h} \Delta f_i + \left(s - \frac{1}{2} \right) \Delta^2 f_i + \left(\frac{3s^2 - 6s + 2}{6} \right) \Delta^3 f_i + \dots$$

Second derivative at non-tabular point x :

$$f''(x) = \frac{d^2}{dx^2} P_n(s) = \frac{d}{dx} \frac{d}{dx} P_n(s) = \frac{d}{dx} \frac{d}{ds} P_n(s) \frac{1}{h} = \frac{1}{h^2} \frac{d^2}{ds^2} P_n(s)$$

$$f''(x) = \frac{1}{h^2} \left(\Delta^2 f_i + (s-1) \Delta^3 f_i + \left(\frac{6s^2 - 18s + 11}{12} \right) \Delta^4 f_i + \dots \right)$$

$$(x) = x_i + sh, \quad \text{at } x = x_i, s = 0$$

$$f'(x_i) = \frac{1}{h} \left[\Delta f_i - \frac{1}{2} \Delta^2 f_i + \frac{1}{3} \Delta^3 f_i + \dots \right]$$

$$f''(x_i) = \frac{1}{h^2} \left[\Delta^2 f_i - \Delta^3 f_i + \frac{11}{12} \Delta^4 f_i + \dots \right]$$

$$S = 1/2, \quad x = x_i + \frac{h}{2} \rightarrow \text{half way point}$$

$$f' \left(x_i + \frac{h}{2} \right) = \frac{1}{h} \left(\Delta f_i - \frac{1}{24} \Delta^3 f_i + \dots \right)$$

$$f'' \left(x_i + \frac{h}{2} \right) = \frac{1}{h^2} \left(\Delta^2 f_i - \frac{1}{3} \Delta^3 f_i + \dots \right)$$

$$S = 1, \quad x = x_i + h, \text{ the next point}$$

$$f' (x_{i+h}) = \frac{1}{h} \left(\Delta f_i + \frac{1}{2} \Delta^2 f_i - \frac{1}{6} \Delta^3 f_i + \dots \right)$$

$$f'' (x_{i+h}) = \frac{1}{h^2} \left(\Delta^2 f_i - \frac{1}{12} \Delta^3 f_i + \dots \right)$$

Truncating at first term only

$$f'(x) = \frac{\Delta f_i}{h} = \frac{f_{i+1} - f_i}{h}$$

$$f''(x) = \frac{\Delta^2 f_i}{h^2} = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2}$$

At tabular points

$$f' (x_i) = \frac{\Delta f_i}{h}, \quad f'' (x_i) = \frac{\Delta^2 f_i}{h^2}$$

At half way point

$$f' \left(x_i + \frac{h}{2} \right) = \frac{\Delta f_i}{h}$$

$$f'' \left(x_i + \frac{h}{2} \right) = \frac{\Delta^2 f_i}{h^2}$$

At next point

$$f'(x_i + h) = \frac{\Delta f_i}{h}$$

$$f''(x_i + h) = \frac{\Delta^2 f_i}{h^2}$$



ACTIVITIES

Example

Estimate $f'(0.1)$ and $f''(0.1)$ from the function $f(x) = e^x$: 0.1 (0.05) 0.3 and determine the accuracy of the result.

Solution

x_i	f_i	$\Delta x 10^{-5}$	Δ^2	Δ^3	Δ^4
0.1	1.10517				
0.15	1.16183	5666			
0.20	1.22140	5957	291	15	-1
0.25	1.28403	6263	306	14	
0.30	1.34986	6583	320		

$$f'(x_i) = \frac{1}{h} \left(\Delta f_i - \frac{1}{2} \Delta^2 f_i + \frac{1}{3} \Delta^3 f_i - \frac{1}{4} \Delta^4 f_i + \dots \right)$$

(Difference is almost constant when $n = 3$)

$$f'(0.1) = \frac{1}{h} (\Delta f_i - \frac{1}{2} \Delta^2 f_i + \frac{1}{3} \Delta^3 f_i)$$

The error generate will be $e = -\frac{1}{4} \frac{\Delta^4 f_i}{h}$

$$f'(0.1) = \frac{1}{0.05} \left(5666 \times 10^{-5} - \frac{1}{2} \times 29 \times 10^{-5} \right) = 1.1051 \text{ (rounded to 4 dp)}$$

$$f''(x_i) = \frac{1}{h^2} (\Delta^2 f_i - \Delta^3 f_i + \frac{11}{12} \Delta^4 f_i + \dots)$$

for $n = 3$

$$f''(0.1) = \frac{1}{h^2} (\Delta^2 f_i - \Delta^3 f_i), \quad e = \frac{11}{12} \Delta^4 f_i \frac{1}{h^2}$$

$$= \frac{1}{(0.005)^2} (291 \times 10^{-5} - 15 \times 10^{-5}) = 1.104 \text{ (bounded to 3 dp)}$$

In the first derivative

$$\text{error} = \frac{-1}{4} \frac{\Delta^4 f_i}{h} = \frac{1}{4 \times (0.05)^{(-1) \times 10^{-5}}} = 0.5 \times 10^{-4}$$

In the second derivative

$$\text{error} \frac{1}{h^2} \times \frac{11}{12} \Delta^4 f_i = \frac{1}{(0.05)^2} \frac{11}{12} (-1) \times 10^{-5} = 0.37 \times 10^{-5}$$



ACTIVITIES

Note: $f(x) = e^x$, $f'(x) = e^x$, $f''(x) = e^x$

$$f(0.1) = f'(0.1) = f''(0.1) = 1.10517$$

$$\text{Error} = 1.10517 - 1.104 = 0.00117$$

Example

Using the following data find $f'(6.0)$, and $f''(6.3)$, $\text{error} = \theta(h^2)$

x	6.0	6.1	6.2	6.3	6.4
$f(x)$	0.1750	-0.1998	-0.2223	-0.2422	-0.2596

Method of $o(h)$ for $f'(x_0)$ is given by

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} \quad f'(6.0) = \frac{f(6.1) - f(6.0)}{0.1} = \frac{-0.1998 - 0.1750}{0.1} = -3.748$$

Method of $O(h^2)$ for $f''(x)$ is

$$f''(x_0) = \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2}$$

$$f''(6.3) = [f(6.2) - 2f(6.3) + f(6.4)] / (0.1)^2 = 0.25$$



SELF-TEST QUESTIONS

- 1) Use the table below to find $f'(1.4)$ and $f''(1.4)$ using $h = 0.1$ and $h = 0.2$

x	1.2	1.3	1.4	1.5	1.6
$f(x)$	1.5095	1.6984	1.9045	2.1293	2.3756

- 2) Prove the relations below

i) $f'(x) = \frac{1}{\Delta} f_0 = \frac{f_1 - f_0}{h}$

ii) $hf'(x_0) = \Delta f_0 - \frac{1}{2} \Delta^2 f_0 + \frac{1}{3} \Delta^3 f_0 \dots \dots \dots$

iii) $hf'(x_0) = \Delta^2 f_0 - \Delta^3 f_0 + \frac{11}{12} \Delta^4 f_0 + \dots \dots \dots$

- 3) Estimate the values of $f'(0.05)$ and $f''(0.05)$ using the data below

x	0.0	0.1	0.2	0.3	0.4
$f(x)$	3.000	2.710	2.440	2.190	1.960



REFERENCES

1. Numerical Analysis: Richard L. Burden, J. Douglas Faires
2. Numerical Methods for Scientific and Engineering Computation: M. K. Jain
3. Numerical Analysis: Schaum's Outline Series
4. Advanced Engineering Mathematics: Arwin Kreyszig.
4. Any other relevant material (text) on Elementary Numerical Analysis.

LECTURE FIVE**NUMERICAL INTEGRATION****5.1 INTRODUCTION**

In Applied Mathematics we are often faced with the problem of differentiating and integrating functions which are defined in a tabular or graphical form rather than explicit functions. Sometimes there are certain explicit functions which are difficult to integrate in terms of elementary functions. In such cases one can resort to numerical integration. In this lesson some methods of numerical integration will be discussed.

**5.2 LECTURE OBJECTIVES**

By the end of this lecture the learner should be able to:

- i) Derive the trapezoidal formula and use it to evaluate integrals.
- ii) Determine the errors arising from using the formula.
- iii) Derive Simpson's rule and use it to evaluate integrals.
- iv) Achieve desired accuracy in numerical integration by using Romberg technique.
- v) Derive and apply the Gaussian quadrature rule for numerical integration.

5.3. Definite and indefinite integrals

The indefinite integral of a function is another function or a class of functions, whereas the definite integral of a function over a fixed interval is a number. For example:

Indefinite integral : $\int x^2 dx = \frac{1}{3}x^3 + C$

$$\text{Definite integral : } \int_0^2 x^2 dx = \frac{1}{3} x^3 \Big|_0^2 = \frac{8}{3}$$

The definite and indefinite integrals are related by the Fundamental Theorem of Calculus which states that $\int_a^b f(x) dx$ can be computed by first finding an anti-derivative $F(x)$ of $f(x)$ and then evaluating $F(b) - F(a)$

$$\int_a^b F'(x) dx = F(b) - F(a)$$

5.4. Trapezoidal rule

Consider the area under the curve $f(x)$ from $x=a$ to $x=b$ divided into n equal strips of width $\frac{b-a}{n} = h$ as in **figure 1** below:

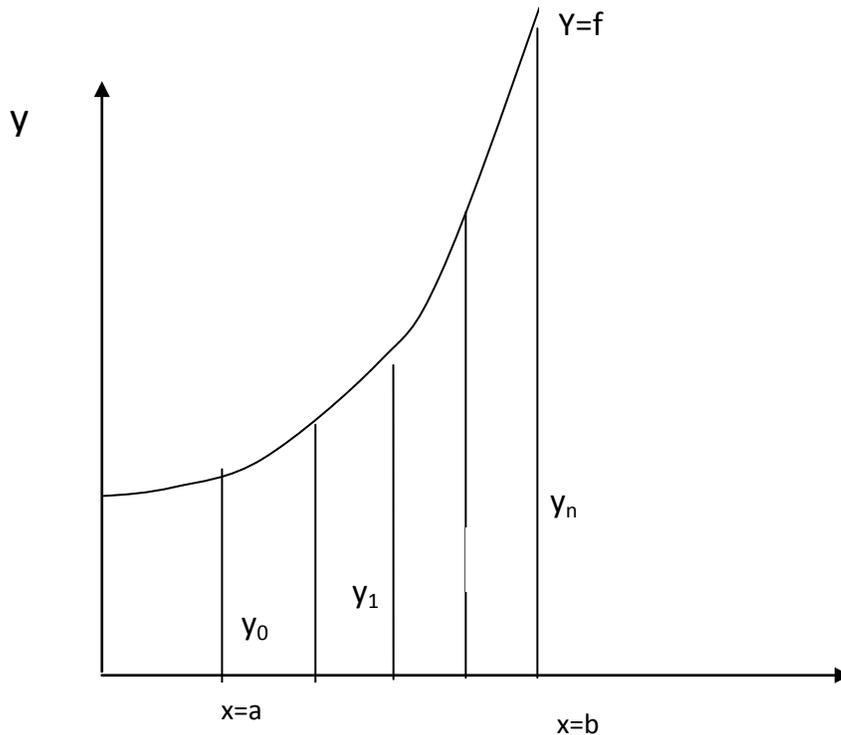


Figure 5.1

To estimate the area $\int_a^b f(x) dx$ we join the tips by straight lines to form trapezia.

Then using the formula: Area of trapezium = $\frac{h}{2} (a + b)$, where $(a + b)$ = sum of parallel sides.

$$\begin{aligned}
 \int_a^b f(x)dx &= h/2 (y_0 + y_1) + h/2 (y_1 + y_2) + \dots + h/2 (y_{n-1} + y_n) \\
 &= h/2 (y_0 + 2y_1 + 2y_2 + \dots + 2y_{n-1} + y_n) \\
 &= h/2 (y_0 + y_n) + 2(y_1 + y_2 + y_3 + \dots + y_{n-1}) \\
 &= h/2 [(sum\ of\ ends) + 2(sum\ of\ middles)]
 \end{aligned}$$

Example

Use the trapezoidal rule with $n = 4$ to estimate $\int_1^2 x^2 dx$

Solution : $n = 4$, $b - a = 1$, $h = 1/4$

X	1.0	1.25	1.5	1.75	2.0
F(x) = x^2	1.0000	1.5625	2.2500	3.0625	4.0000
	y_0	y_1	y_2	y_3	y_4

$$\int_a^b x^2 dx = 1/2 \times 1/4 (1 + 4) + 2(1.5625 + 2.25 + 3.0625) = 2.3438 (4dp)$$

Comparing with the exact solution

$$\int_1^2 x^2 dx = \left[\frac{x^3}{3} \right]_1^2 = \frac{8}{3} - \frac{1}{3} = \frac{7}{3} = 2.3333$$

The area from trapezoidal rule is an over estimate. The error can be reduced by using smaller strips. For example if 8 strips are used then $h = 1/8$

x	1.000	1.125	1.250	1.375	1.500	1.625	1.750	1.875	2.000
F(x)	1.000	1.2656	1.5625	1.890625	2.25	2.640625	3.0625	3.51625	4.000

2

$$\int_1^2 x^2 dx = \frac{1}{2}x^2 \Big|_1^2 = \frac{1}{2}(4 - 1) = \frac{3}{2} = 1.5$$

2.3359 (4dp)

5.5. Error in Trapezoidal rule

$$R_n = \frac{1}{(n+1)!} \int_a^b w(x) \Pi(x) f^{(n+1)}(\xi) dx$$

setting $x = x_0 + sh$

$$\Pi(x) = h^{n+1} s(s-1)(s-2) \dots (s-n)$$

$$R_n = \frac{h^{n+2}}{(n+1)!} \int_0^1 s(s-1)(s-2) \dots (s-n) f^{(n+1)}(\xi) ds$$

$$R_1 = \frac{h^3}{2} \int_0^1 s(s-1) f''(\xi) ds$$

 $s(s-1)$ does not change sign in the interval $[0,1]$, we get

$$R_1 = \frac{h^3}{2} f''(\eta) \int_0^1 s(s-1) ds, \quad \eta \in [0,1] = \frac{h^3}{2} f''(\eta) \left[\frac{s^3}{3} - \frac{s^2}{2} \right]_{s=0}^{s=1}$$

$$= \frac{h^3}{2} f''(\eta) \left(-\frac{1}{6} \right) = -\frac{h^3}{12} f''(\eta). \text{ But } h = (b-a)$$

$$R_1 = -\frac{h^3}{12} (b-a) f''(\eta), \text{ which can be written as : } |E_T| \leq h^2 \frac{(b-a)}{12} M$$

where M is the maximum value of f'' on $[a, b]$.



ACTIVITIES

If the trapezoidal rule is used to compute $\int_0^1 e^{-x^2} dx$ with an error of at most 0.0005, how many points should be used?

Solution :

$$f(x) = e^{-x^2}, f'(x) = -2x e^{-x^2}, f''(x) = (4x^2 - 2)e^{-x^2}$$

$$f''(0) = 2, \quad f''(1) = \frac{2}{e}$$

$$|E_T| \leq h^2 \frac{(b-a)}{12} f''(\epsilon) = \frac{h^2(1)}{12} \cdot 2 < 0.00005$$

$$h^2 < (0.00005 \times 6), \quad h < \sqrt{0.0003}, \quad h < 0.01732$$

$$n = \frac{b-a}{h} = \frac{1}{0.01732} = 57.7 \approx 58$$

The strips are 58 and hence the points are 59.



SELF-TEST QUESTIONS

1. Many sub intervals are needed to approximate $\int_0^1 \frac{\sin x}{x} dx$

With error not exceeding 0.5×10^{-5} using the trapezoidal rule?

2. Find the maximum error in evaluating $\int_1^2 x^2 dx$ with $h = \frac{1}{4}, \frac{1}{8}, \frac{1}{16}$,

comment on the results.

5.6. Simpson's rule

The Simpson's rule gives a formula for an estimate of the area under the portion of a curve between a and b in terms of three ordinates y_0, y_1 and y_2 . Consider the area under the curve $y=f(x)$ as in figure 5.2 below

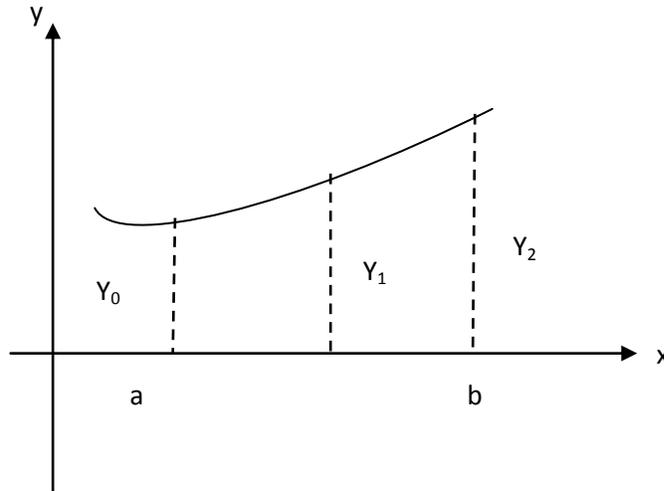


Figure 5.2

By translation we could have the same area as in figure 5.3 below

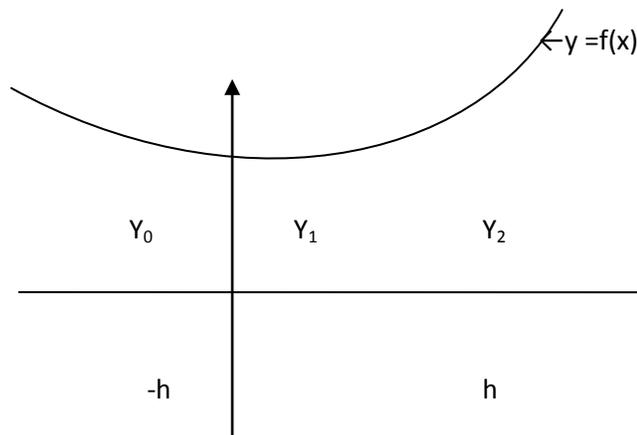


Figure 5.3

To approximate $f(x)$ over $[-h, h]$ by a parabola we have the required area as

$$\int_{-h}^h (ax^2 + bx + c) dx = \left[\frac{ax^3}{3} + \frac{bx^2}{2} + cx \right]_{-h}^h = \left[\frac{ah^3}{3} + \frac{bh^2}{2} + ch \right] - \left[\frac{ah^3}{3} + \frac{bh^2}{2} + ch \right]$$

$$= \frac{2}{3}ah^3 + 2ch = \frac{h}{3}(2ah^2 + 6c)$$

From the figure (5.3),

$$y_0 = ah^2 - bh + c \text{ for } x = -h, y_1 = c \text{ for } x = 0$$

$$y_2 = ah^2 + bh + c \text{ for } x = h$$

$$\frac{h}{3}(2ah^2 + 6c) = \frac{h}{3}(2ah^2 + 2c + 4c) = \frac{h}{3}(y_0 + y_2 + 4y_1)$$

Considering the are under $f(x)$ from $x = a$ to $x = b$

$$\begin{aligned} \int_a^b f(x) &= \frac{h}{3} [y_0 + y_1 + y_2] + \frac{h}{3} (y_2 + 4y_3 + y_4) + \frac{h}{3} (y_4 + 4y_5 + y_6) + \dots \\ &+ \frac{h}{3} (y_{n-2} + 4y_{n-1} + y_n) \\ &= \frac{h}{3} (y_0 + y_n) + 2(y_2 + y_4 + y_6 + \dots + y_{n-2}) + 4(y_1 + y_3 + \dots + y_{n-1}) \end{aligned}$$

which can be summarized as:

$$\frac{h}{3} (\text{sum of ends} + 4(\text{sum of odd strips}) + 2(\text{sum of even strips}))$$



ACTIVITIES

A particle moves along a straight line so that at time t its distance s from a fixed point of the line is given by

$$\frac{ds}{dt} = t(\sqrt{8 - t^3})$$

Use the Simpsons rule with 8 strips to calculate the approximate distance travelled by the particle from $t=0$ to $t=2$

Solution

$$\frac{ds}{dt} = t(\sqrt{8 - t^3})$$

$$s = \int_0^2 t(\sqrt{8-t^3}) dt$$

t	0	0.25	0.5	0.75	1.0	1.25	1.50	1.75	2.00
$\frac{ds}{dt}$	0	0.706	1.403	2.065	2.646	3.074	3.225	2.847	0.0

By Simpson's rule

$$\begin{aligned}
 s &= \frac{0.25}{3} ((0 + 0) + 4(0.706 + 2.065 + 3.074 + 2.847) + 2(1.403 + 2.64 + 3.225)) \\
 &= \frac{0.25}{3} (4(8.689) + 2(7.2)) = 4.108
 \end{aligned}$$



ACTIVITIES

Estimate $\int_1^2 x^2 dx$ using the Simpson's rule with $n = 4$

$$\begin{aligned}
 A &= \frac{1}{2} x \frac{1}{4} (5 + 2(2.25) + 4(1.5625 + 3.065)) \\
 &= \frac{1}{12} (5 + 4.5 + 18.51) = \frac{28.1}{12} = 2.3342 \text{ (4dp)}
 \end{aligned}$$

5.7. Error in Simpson's rule

The maximum error possible using Simpson's rule satisfies

$$|E_s| \leq \frac{(b-a)h^4 M}{180}$$

Where M is the maximum $f^{(iv)}$ on $[a, b]$, $[f^{(iv)}$ is the fourth derivative]



ACTIVITIES

Estimate the maximum error in $\int_0^1 5x^4 dx$ using Simpson's rule with $n=4$.

Solution:

$$f(x) = 5x^4, f'(x) = 20x^3, f''(x) = 60x^2, f'''(x) = 120x, f^{(iv)}(x) = 120$$

$$M = \max f^{(iv)} \text{ on } [0,1] = 120$$

$$|E_S| = \frac{1 \times \left(\frac{1}{16}\right)^2 \times 120}{180} = 0.002604$$



ACTIVITIES

Using the trapezoidal and Simpson's rules approximate the value of $\int_0^1 x \ln(x+1) dx$ using 9 (nine) ordinates. Compare your results with the exact solution correct to five significant figures

Solution

$$h = \frac{1-0}{8} = \frac{1}{8}$$

$$y_0 = 0 \ln(0+1) = 0.00000$$

$$y_1 = \frac{1}{8} \ln\left(1 + \frac{1}{8}\right) = 0.014723$$

$$y_2 = \frac{2}{8} \ln\left(1 + \frac{2}{8}\right) = 0.05579$$

$$y_3 = \frac{3}{8} \ln\left(1 + \frac{3}{8}\right) = 0.11942$$

$$y_4 = \frac{4}{8} \ln\left(1 + \frac{4}{8}\right) = 0.20273$$

$$y_5 = \frac{5}{8} \ln\left(1 + \frac{5}{8}\right) = 0.30344$$

$$y_6 = \frac{6}{8} \ln\left(1 + \frac{6}{8}\right) = 0.45962$$

$$y_7 = \frac{7}{8} \ln \left(1 + \frac{7}{8} \right) = 0.55003$$

$$y_8 = \frac{8}{8} \ln \left(1 + \frac{8}{8} \right) = 0.69315$$

By trapezoidal rule

$$\int_0^1 f(x) = \frac{1}{8} (0.0000 + 0.69315) + 2(1.66584) = \frac{1}{16} (4.02483) = 0.25155$$

By Simpson's rule

$$\int_0^1 f(x) = \frac{1}{8} (0.0000 + 0.69315) + 4 + 2(0.67823) = \frac{1}{24} (6.00005) = 0.2500$$

Exact solution can be obtained by integration by parts

$$\text{Let } U = \ln(x+1), \quad V' = x, \quad U = \ln \frac{1}{x+1}, \quad V = x^2/2$$

$$\begin{aligned} \int_0^1 x \ln(x+1) dx &= \frac{x^2}{2} \ln(x+1) - \left[\frac{1}{2} \left[\frac{x^2}{2} - x + \ln(x+1) \right] \right]_0^1 \\ &= \left[\frac{1}{2} \ln 2 - \frac{1}{4} + \frac{1}{2} - \frac{1}{2} \ln 2 \right] = \frac{1}{2} - \frac{1}{4} = \frac{1}{4} = 0.2500 \end{aligned}$$

Error in Trapezoidal rule = 0.00155

Error in Simpson's rule = 0.00000

Hence Simpson's approximation is more accurate than Trapezoidal rule in this case.

5.8. Tabular data

Numerical integration can be used to approximate the integral of a function described in tabular form. In this case it is not possible to determine the error since the function is not known.



ACTIVITIES

Suppose it is found experimentally that two physical variables x and y are related as shown in the table below

x	1.0	1.5	2.0	2.5	3.0	3.5	4.0
y	3.1	4.0	4.2	3.8	2.9	2.8	2.7

${}^4\int_1 f(x)dx$ can be calculated by follows :

$$\text{Trapezoid rule} = \frac{0.5}{2} ((3.1 + 2.7) + 2(4.0 + 4.2 + 3.8 + 2.9 + 2.8)) = 10.3$$

$$\text{Simpson's rule} = \frac{0.5}{2} ((3.1 + 2.7) + 4(4.0 + 3.8 + 2.8) + 2(4.2 + 2.9)) = 10.4$$



SELF-TEST QUESTIONS

1. Use trapezoidal and Simpson's rules to approximate the given integrals for the stated values of n . Hence Estimate the error in each case

$$4 \int_1^{\frac{1}{x}} dx, n = 6$$

i. $\int_0^3 \frac{dx}{1+x}, n = 8$

ii. $3 \int_2^{\sqrt{1+x^3}} dx, n = 4$

2. a) How large must n be if the trapezoidal rule is to estimate

$$2 \int_5 e^{-x^2} dx \text{ with an error not exceeding } 10^{-6}$$

- b) If Simpson's rule is used to compute

$$\int_0^1 \frac{1}{1+x} dx \text{ with an error of at most } 10^{-6} \text{ how many points should be used?}$$

3. Using trapezoidal and Simpson's rules, find $\int_2^4 f(x) dx$ from the data below

X	2.0	2.25	2.50	2.75	3.00	3.25	3.50	3.75	4.0
F(x)	4.12	3.76	3.21	3.58	3.94	4.15	4.69	5.44	7.52

5.9. Newton cotes and Composite formulae

The Trapezoidal rule and Simpson's rule are examples of a class of methods known as Newton -cotes formulae. They are used to approximate the integral

$$I = \int_a^b W(x)f(x) dx$$

where $W(x)=1$ and the nodes x_i are equally spaced with $x_0 = a$, $x_n = b$ and spacing $h = \frac{b-a}{n}$

However Newton-cotes formula are generally unsuitable for use over large integration intervals and where the nodes are not equally spaced.

The composite Trapezoidal rule

The composite formula is obtained by applying the simple formula to cover longer intervals by subdividing the given interval. The interval $[a,b]$ is subdivided into n intervals of length

$h = \frac{(b-a)}{n}$. Denoting the sub-intervals as $(x_0, x_1), (x_1, x_2), (x_2, x_3) \dots \dots \dots$
 (x_{n-1}, x_n) where $x_0 = a, x_n = b$

$x_i = x_0 + ih$, we write

$$I = \int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \dots \dots \dots + \int_{x_{n-1}}^{x_n} f(x)dx$$

Evaluating each of the integrals on the right hand side of the above equation by trapezoidal rule, we obtain

$$I = \frac{h}{2} [(f_0 + f_1) + (f_1 + f_2) + \dots \dots \dots + (f_{n-1} + f_n)]$$

$$= \frac{h}{2} [(f_0 + f_n) + 2(f_1 + f_2 \dots \dots + f_{n-1})]$$

Generally composite integration involves a piecewise integration.

$$T(f, h) = \frac{h}{2} [f(a) + f(b)] + h \sum_{K=1}^{M-1} f(x_K)$$



ACTIVITIES

Evaluate the integral $I = \int_0^1 \frac{dx}{1+x}$ using composite trapezoidal rule with 2,4, and

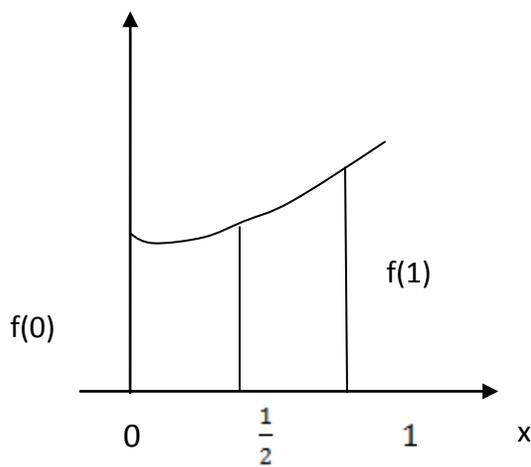
8 equal subintervals

Solution

i) when $n=2$, $h = \frac{1}{2} = 0.5$

$$T = \left(f, \frac{1}{2}\right) = \frac{0.5}{2} \left[f(0) + f(1) + 2f\left(\frac{1}{2}\right) \right]$$

$$= \frac{1}{4} \left(1 + \frac{4}{3} + \frac{1}{2} \right) = \frac{17}{24} = 0.708333$$



ii) when $n=4$, $h = \frac{1}{4}$, each strip is further divided into two

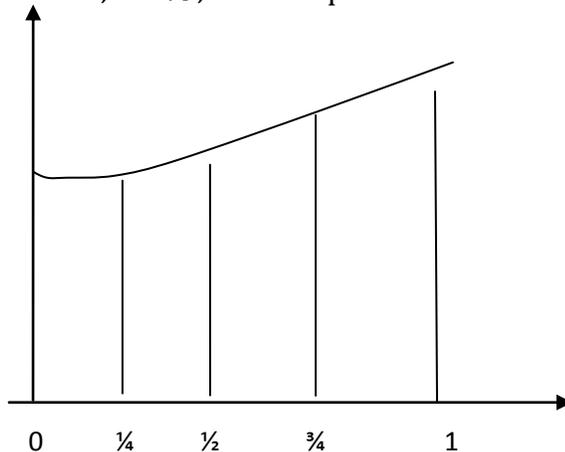


Figure 5.5

$$T \left(f, \frac{1}{4} \right) = \frac{0.25}{2} \left(f(0) + f(1) + 2 \left[f\left(\frac{1}{4}\right) + f\left(\frac{1}{2}\right) + f\left(\frac{3}{4}\right) \right] \right) = 0.697024$$

iii) when $n=8$, $h = 1/8$

$$T\left(f, \frac{1}{8}\right) = \frac{1}{16} \left(f(0) + f(1) + 2 \sum_{i=1}^7 f\left(\frac{i}{8}\right) \right) = 0.694122$$

The exact integral is: $I = \int_0^1 \frac{dx}{1+x} = \ln(1+x)|_0^1 = 0.693147$

5.10. Romberg integration

Romberg integration uses the composite Trapezoidal rule to give preliminary approximations and then applies Richardson extrapolation process to improve the approximations. Romberg algorithm produces a triangular array of numbers all of which are numerical estimates of the definite integral $\int_a^b f(x)dx$.

The array can be denoted by

$$T_1^0$$

$$T_2^0 \quad T_2^1$$

$$T_3^0 \quad T_3^1 \quad T_3^2$$

$$T_4^0 \quad T_4^1 \quad T_4^2 \quad T_4^3$$

$$T_5^0 \quad T_5^1 \quad T_5^2 \quad T_5^3 \quad T_5^4$$

The first column contains estimates of the integral obtained by composite (recursive) trapezoidal formula. The first term is obtained with just one trapezium, second term with two trapezia, third term with four trapezia and so on. Extrapolation for the other columns is done using the formula

$$T_k^i = \frac{4^i T_k^{i-1} - T_{k-1}^{i-1}}{4^i - 1}$$



ACTIVITIES

Find the approximate value of the integral $\int_1^2 \frac{1}{x} dx$ using Romberg integration with $n = 16$.

Solution

First we compute the trapezoidal approximations starting with $n = 2$ and doubling n each time. A table for values to be used may be constructed as below with

$$h = \frac{2 - 1}{16} = \frac{1}{16} = 0.0625$$

X	1.0	$\frac{17}{16}$	$\frac{18}{16}$	$\frac{19}{16}$	$\frac{20}{16}$	$\frac{21}{16}$	$\frac{22}{16}$	$\frac{23}{16}$	$\frac{24}{16}$	$\frac{25}{16}$	$\frac{26}{16}$	$\frac{27}{16}$	$\frac{28}{16}$	$\frac{29}{16}$	$\frac{30}{16}$	$\frac{31}{16}$	2.0
f(x)	1.0	$\frac{16}{17}$	$\frac{16}{18}$	$\frac{16}{19}$	$\frac{16}{20}$	$\frac{16}{21}$	$\frac{16}{22}$	$\frac{16}{23}$	$\frac{16}{24}$	$\frac{16}{25}$	$\frac{16}{26}$	$\frac{16}{27}$	$\frac{16}{28}$	$\frac{16}{29}$	$\frac{16}{30}$	$\frac{16}{31}$	0.5

When:

$$n = 1 : T_0^1 = \frac{1}{2} \left(1 + \frac{1}{2} \right) = 0.75$$

$$n = 2 : T_0^2 = \frac{0.5}{2} \left(\frac{3}{12} + 2 \left(\frac{2}{3} \right) \right) = 0.7083333$$

$$n = 4 : T_3^0 = \frac{0.25}{2} \left(1.5 + 2 \left(\frac{1}{2.5} + \frac{1}{1.5} + \frac{1}{1.75} \right) \right) = 0.6970238$$

$$n = 8 : T_4^0 = 0.69412185$$

$$n = 16 : T_5^0 = 0.69314718$$

Using the extrapolation formula

$$T_k^i = \frac{4^i T_k^{i-1} - T_{k-1}^{i-1}}{4^i - 1}$$

We compute the other columns

$$T_2^1 = \frac{4T_2^0 - T_1^0}{3} = 0.69444444$$

$$T_3^1 = \frac{4T_3^0 - T_2^0}{3} = 0.693253$$

$$T_3^2 = \frac{16T_3^1 - T_2^1}{15} = 0.6931746$$

and so on. Every entry depends only on its left and left-top neighbor. Continuing in this way, we get the following table

0.7500000				
0.7083333	0.6944444			
0.6970238	0.6932539	0.6931746		
0.6941219	0.6931545	0.6931479	0.6931474	
0.69333391	0.6931476	0.6931471	0.6931472	0.6931472

The exact answer is $\ln 2 = 0.69314718$ correct to 8 decimal places.

The error at each stage of integration is given by $T_i^k - \ln 2$ which reduces on successive extrapolations or iteration.



SELF-TEST QUESTIONS

Use four iterations of Romberg integration to estimate $\pi = \int_0^1 \frac{4}{1+x^2} dx$.

Comment on the accuracy of your results

5.11. Methods based on undetermined coefficients and quadrature formula

There is a large family of numerical integration formulae that conform to the pattern

$$\int_a^b f(x)dx = A_1f(x_1) + A_2f(x_2) + \dots + A_n f(x_n) \quad \text{----- (1)}$$

In using this it is only necessary to know the nodes x_1, x_2, \dots, x_n and the “weights” A_1, A_2, \dots, A_n . There are tables in which the numerical values of the nodes and weights are listed. However they can be derived.

Theorem: Let q be a polynomial of degree n such that

$\int_a^b f(x) x^k dx = 0$, $k = 0, 1, 2, \dots, n-1$, let x_1, x_2, \dots, x_n be the roots of q . Then

$$\int_a^b f(x) dx = \int_a^b P(x) dx = \sum_{i=1}^n f(x_i) \int_a^b \ell_i(x) dx = \sum_{i=1}^n A_i f(x_i) \dots \dots (2)$$

will be exact for all polynomials of degree $\leq 2n - 1$



ACTIVITIES

Determine the Gaussian quadrature formula with three Gaussian nodes and three weights for the integral $\int_{-1}^1 f(x) dx$

Solution:

We first find the polynomial $q(x)$ required and its roots. For degree 3

$$\text{Let } q(x) = C_0 + C_1 x + C_2 x^2 + C_3 x^3$$

$q(x)$ must satisfy the condition

$$\int_{-1}^1 q(x) dx = \int_{-1}^1 x q(x) dx = \int_{-1}^1 x^2 q(x) dx = 0$$

$$\text{If } C_0 = C_2 = 0 \text{ then } q(x) = C_1 x + C_3 x^3 \text{ and so } \int_{-1}^1 q(x) dx = \int_{-1}^1 x^2 q(x) dx = 0$$

because the integral of an odd function over a symmetric interval is 0 (Zero). In order to obtain c_1 and c_3 we impose the condition

$$\int_{-1}^1 x(c_1 x + c_3 x^3) dx = 0$$

A convenient solution of this is $C_1 = \frac{-3}{2}$ and $C_3 = \frac{5}{3}$. Hence

$$q(x) = \frac{5}{2} x^3 - \frac{3}{2} x = x \left(\frac{5}{2} x^2 - \frac{3}{2} \right). \text{ The roots of } q \text{ are } -\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}.$$

These are the Gaussian nodes for the quadrature formula.

To obtain the weights A_1, A_2 and A_3 we use a procedure known as “Method of undetermined coefficients”. We want to determine A_1, A_2 and A_3 in the formula

$$\int_{-1}^1 f(x) dx = A_1 f\left(-\sqrt{\frac{3}{5}}\right) + A_2 f(0) + A_3 f\left(\sqrt{\frac{3}{5}}\right) \quad (3)$$

so that the approximate equality is an exact whenever f is of the form

$ax^2 + bx + c$. Eqn—(3) will be exact for all polynomials of degree ≤ 2 if it is exact for $1, x$ and x^2

Arranging in a tabular form

f	<i>L.H.S.</i>	<i>R.H.S.</i>
1	$\int_{-1}^1 dx = 2$	$A_1 + A_2 + A_3$
x	$\int_{-1}^1 x dx = 0$	$-\sqrt{\frac{3}{5}}A_1 + \sqrt{\frac{3}{5}}A_3$
x^2	$\int_{-1}^1 x^2 dx = \frac{2}{3}$	$\frac{3}{5}A_1 + \frac{3}{5}A_3$

Solving

$$A_1 + A_2 + A_3 = 2$$

$$A_1 - A_3 = 0$$

$$A_1 + A_3 = \frac{10}{9} \text{ we obtain } A_1 = A_3 = \frac{5}{9}, A_2 = \frac{8}{9}$$

Therefore the formula is

$$\int_{-1}^1 f(x) dx = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$$

$$= \frac{1}{9} \left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right) \right]$$

This formula is called the Gauss-Legendre 3-point formula or the 3-point Gaussian quadrature formula.

A Gaussian quadrature rule for the interval $[-1,1]$ can be used on the interval, $[a,b]$ by applying a suitable linear transformation. In this case we can transform the interval $[a,b]$ into $[-1,1]$ using the transformation:

$$x = \left(\frac{b-a}{2}\right)t + \left(\frac{b+a}{2}\right)$$

$$\text{giving } \int_{-2}^1 w(x)f(x)dx = \sum_{k=0}^n A_k f(x_k)$$



ACTIVITIES

Evaluate the integral

$$I = \int_{-1}^1 (1-x^2)^{3/2} \cos x \, dx \text{ using Gauss - Legendre three point formula.}$$

Solution

By formula

$$\int_{-1}^1 f(x)dx = \frac{1}{9} \left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right) \right]$$

here $f(x) = (1-x^2)^{3/2} \cos x$. Hence,

$$I = \frac{2}{9} \left[1 \sqrt{\frac{2}{5}} \cos \sqrt{\frac{3}{5}} + 4 + \sqrt{\frac{2}{5}} \cos \sqrt{\frac{3}{5}} \right] = 1.08979$$



ACTIVITIES

Evaluate $I = \int_0^1 \frac{1}{1+x} dx$ using Gaussian quadrature 3 point formula

Solution

First we convert the integral to $[-1, 1]$ from $[0, 1]$

$$\text{Let } x = \left(\frac{b-a}{2}\right)t + \left(\frac{b+a}{2}\right)$$

$$x = \left(\frac{1-0}{2}\right)t + \left(\frac{1+0}{2}\right) = \frac{1}{2}t + \frac{1}{2}, \quad dx = \frac{1}{2}dt$$

$$\int_0^1 \frac{1}{1+x} dx = \int_{-1}^1 \left(\frac{\frac{1}{2}dt}{1+\frac{1}{2}(t+1)}\right) = \int_{-1}^1 \left(\frac{dt}{t+3}\right), \text{ with } f(t) = \frac{1}{t+3}$$

Using the formula:

$$\int_{-1}^1 f(x) dx = \frac{1}{9} \left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right) \right] = \frac{1}{9} \left[\frac{3}{-\sqrt{\frac{3}{5}+3}} \frac{8}{3} + \frac{5}{\sqrt{\frac{3}{5}+3}} \right] = 0.693122$$

Comparing with exact value :

$$\int_0^1 \frac{1}{1+x} dx = \ln(1+x) \Big|_0^1 = 0.69314718 \text{ (8dp)}$$



SELF-TEST QUESTIONS

Use the Gauss-Legendre 3-point formula to evaluate the following:

$$1) \int_{-1}^1 x^6 dx \quad 2) \int_{-1}^1 \frac{2x}{1+x^4} dx \quad 3) \int_{-1}^1 e^{-x^2} \cos x dx$$

$$4) \int_{-1}^1 \frac{\cos 2x}{1 + \sin x} dx$$

**REFERENCES**

1. **Numerical Analysis: Richard L. Burden, J. Douglas Faires**
2. **Numerical Methods for Scientific and Engineering Computation: M. K. Jain**
3. **Numerical Analysis: Schaum's Outline Series**
4. **Advanced Engineering Mathematics: Arwin Kreyszig.**
4. **Any other relevant material (text) on Elementary Numerical Analysis.**

LECTURE SIX

ITERATION TECHNIQUES



6.1 INTRODUCTION

In this chapter the solution techniques to find the roots of a non-linear equation are discussed with reference to practical examples.



6.2 LECTURE OBJECTIVES

By the end of this lecture the learner should be able to:

- i) Define a root of a non-linear equation.
- ii) Use the bisection method to approximate a root of an equation.
- iii) Use the Regular Falsi method for root finding.
- iv) Use the Newton-Raphson method for root finding.
- v) Use the Aitken's formula for accelerating the convergence of the iterative method.

6.3 Direct and indirect iterative methods

A problem of great importance in Applied Mathematics and Engineering is that of determining the roots of an equation of the form $f(x) = 0$.

The function $f(x)$ may be written explicitly as

$$f(x) = P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0$$

where $P_n(x)$ is a polynomial of degree n in x . the function $f(x)$ may be known only implicitly as a transcendental function.

A number r is a solution of $f(x) = 0$ if $f(r) = 0$ and such a solution is called a root or a zero of $f(x) = 0$. Geometrically $y = f(x)$ intersects the x -axis at the root and a function may have a multiple roots.

There are two methods of finding zeroes or roots of $f(x) = 0$

i) **Direct methods**

These methods give the exact value of the roots in a finite number of steps for example solution of the quadratic equation $ax^2 + bx + c = 0$ which is

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

ii) **Iterative methods**

These methods are based on the idea of successive approximations. Starting with one or more initial approximation(s) to the root, we obtain a sequence of approximates or iterates which in the limit converge to the root.

Convergence: A sequence of iterates (x_k) is said to converge to the root ε

$$\lim_{k \rightarrow \infty} |x_k - \varepsilon| = 0$$

If x_k and x_{k+1} are two consecutive iterates then

$|x_{k+1} - x_k| < \varepsilon$, where ε is the prescribed error tolerance. This may be used as a stopping criteria.

6.4. The Bisection method

This technique is based on the intermediate value Theorem (IVT). Suppose f is a continuous function defined on $[a, b]$ with $f(a)$ and $f(b)$ of opposite sign. By the IVT there exists a number p in (a, b) with $f(p) = 0$. We assume that the root in this interval is unique. The method calls for a repeated halving (bisecting) of sub intervals of (a, b) and at each step locating the half containing p .

To begin, set $a_1 = a$ and $b_1 = b$ and let P_1 be the mid point of $[a, b]$ thus

$$P_1 = a_1 + \frac{b_1 - a_1}{2} = \frac{a_1 + b_1}{2}$$

If $f(p) = 0$ then $p = p_1$ and we are done.

If $f(p_1) \neq 0$, then $f(p)$ has the same sign as either $f(a_1)$ or $f(b_1)$

When $f(p_1)$ and $f(a_1)$ have the same sign, $P \in (p_1, b_1)$ and we set $a_2 = p_1$ and $b_2 = b_1$

When $f(p_1)$ and $f(a_1)$ have opposite signs $P \in (a_1, p_1)$ and we set $a_2 = a_1$, $b_2 = p_1$

we reapply the process to the intervals $[a_2, b_2]$.

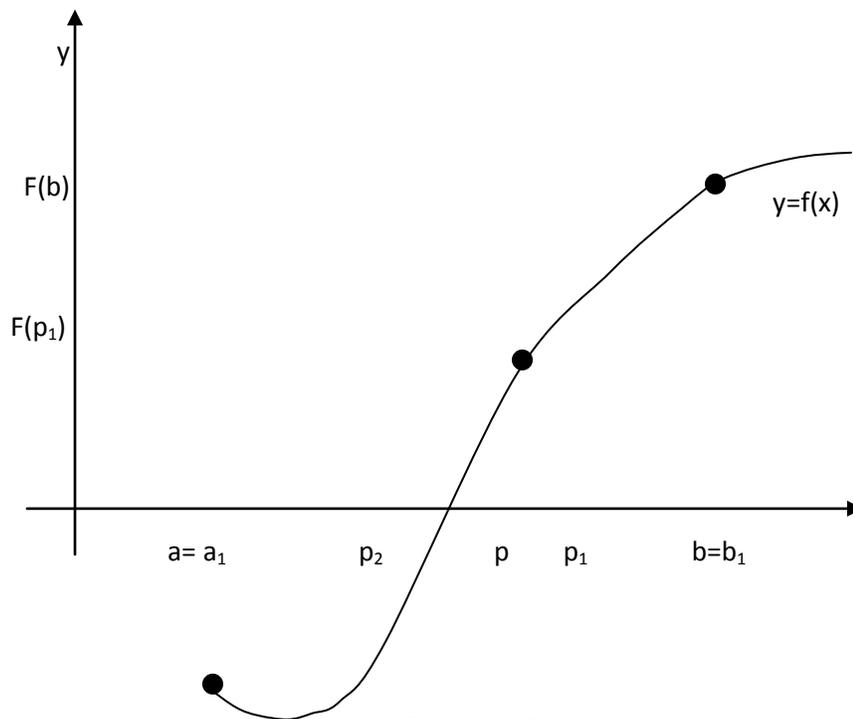


Figure 6.1

Other stopping procedures can be applied for example we can select a tolerance $\varepsilon > 0$ and generate P_1, P_2, \dots, P_N under a condition is met

$$\frac{|P_N - P_{N-1}|}{|P_N|} < \varepsilon, P_N \neq 0$$

$$|f(P_N)| < \varepsilon$$



ACTIVITIES

Perform five iterations of the bisection method to obtain the smallest positive root of the equation $f(x) = x^3 - 5x + 1 = 0$

Solution

Since $f(0) > 0$ and $f(1) < 0$, the smallest positive root lies in the interval $(0,1)$

Taking $a_0 = 0$, $b_0 = 1$ we get $P_1 = \frac{1}{2}(0 + 1) = 0.5$

$$f(P_1) = 0.5^3 - 5(0.5) + 1 = -1.375$$

$$f(a_0) f(P_1) = 1(-1.375) < 0$$

Thus the root lies in the interval $(0, 0.5)$. the sequence of intervals are given in the table below

K	a_{k-1}	b_{k-1}	m_k	$f(m_k)$	$f(a_{k-1})$
1	0	1	0.5	<	0
2	0	0.5	0.25	<	0
3	0	0.25	0.125	>	0
4	0.125	0.25	0.1875	>	0
5	0.1875	0.25	0.21875	<	0

Hence the root lies between $(0.1875, 0.21875)$

**SELF-TEST QUESTIONS**

Use the Bisection method to find solutions accurate to 10^{-2} for

i) $x^3 - 7x^2 + 14x - 6 = 0$ on $[0,1]$,

ii) $x - 2^{-x} = 0$ on $[0,1]$

iii) $e^x - x^2 + 3x - 2 = 0$ on $[0,1]$

iv) $x \cos x - 2x^2 + 3x - 1 = 0$ for $[0.2, 0.3]$, $[1.2, 1.3]$

6.5 Secant method and Regula falsi

if x_{k-1} and x_k are two approximations to the root of the equation $f(x) = 0$ then we determine $a_0x + a_1 = 0$ using the conditions

$$f_{k-1} = a_0 x_{k-1} + a_1$$

$$f_k = a_0 x_k + a_1$$

$$f_{k-1} = f(x_{k-1}) \text{ and } f_k = f(x_k)$$

Solving

$$a_0 = \frac{(f_k - f_{k-1})}{(x_k - x_{k-1})}$$

$$a_0 = \frac{x_k f_{k-1} - x_{k-1} f_k}{(x_k - x_{k-1})}$$

The next approximation

$$x_{k+1} = \frac{x_{k-1} f_k - x_k f_{k-1}}{f_k - f_{k-1}}$$

$$\text{or } x_{k+1} = x_k - \frac{x_k - x_{k-1}}{f_k - f_{k-1}} f_k$$

where $k = 1, 2, \dots, n$.

For example

$$x_2 = x_1 - \frac{x_1 - x_0}{f_1 - f_0} (f_1)$$

$$x_3 = x_2 - \frac{x_2 - x_1}{f_2 - f_1} (f_2)$$

Geometrically, in this method we replace the function $f(x)$ by a straight line or a chord passing through (x_k, f_k) and (x_{k-1}, f_{k-1}) . We then take the point of intersection of the chord with the x axis as the next approximation.

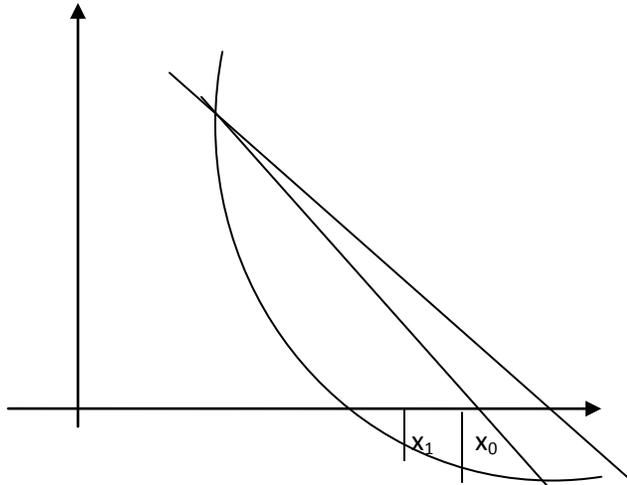


Figure 6.2

If the approximations are such that $f_k f_{k-1} < 0$ the method is known as Regula-Falsi method.



ACTIVITIES

solve $x^3 - 5x + 1 = 0$ using the secant method. Perform 3 iterations.

Solution

Taking the interval $[0,1]$, $f(0) = 1$ $f(1) = -3$

Let $x_0 = 0, x_1 = 1$

$$x_2 = x_1 - \frac{[x_1 - x_0]}{f_1 - f_0} f_1 = 1 - \left(\frac{1 - 0}{-3 - 1} \right) (-3) = 1 - \frac{3}{4} = 0.25$$

$$x_3 = x_2 - \frac{(x_2 - x_1)}{f_2 - f_1} f_2$$

$$\frac{0.25 - (-0.75)}{-15/64 - 3} = \frac{1}{187/64} = \frac{64}{187} = 0.34225$$



ACTIVITIES

Solve $x^3 - 9x + 1$ by Regula Falsi

Solution

Let $x_1 = 2$, $x_2 = 4$

$$f(x_1) = -9, \quad f(x_2) = 29$$

$$x_3 = x_2 - \frac{(x_2 - x_1)}{f(x_2) - f(x_1)} f(x_2) = 4 - \frac{(4 - 2)}{29 - (-9)} = 4 - \frac{2}{38} (29) = 2.47368$$

$$f(x_3) = 15.13 - 22.263 + 1 = -6.13$$

$f(x_2) f(x_3) < 0$, choosing x_2 and x_3

$$x_4 = \frac{2.47368 (29) - 2(-6.13)}{35.13} = 2.73989$$

Proceeding in this manner finally the method converges to 2.97281



SELF-TEST QUESTIONS

Use secant method to solve the equations below over the given intervals and accurate to 10^{-4}

i) $x^3 + 3x^2 - 1 = 0, [-3, -2]$

ii) $e^x - 3x^2 = 0 [0,1], [3,5]$

iii) $x^3 - \cos x [-1,0]$

6.6. Newton-Raphson method

This is the best method for finding successively better approximations to zeroes (or roots) of a real valued function. It converges quickly if the iteration begins sufficiently near the desired root. In Newton –Raphson’s method it is assumed that the function $f(x)$ is differentiable and has a definite slope at each point and hence a unique tangent.

At a certain point $(x_0, f(x_0))$ on the graph f there is a tangent such that

$\ell(x) = f'(x_0)(x - x_0) + f(x_0)$ is close to f near x_0

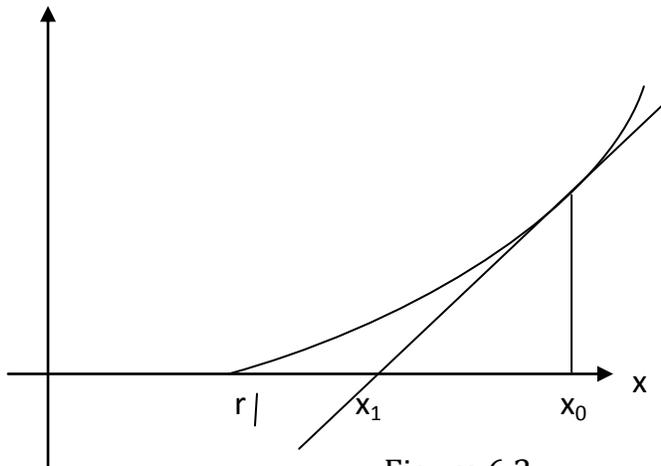


Figure 6.3

We take the zero of 1 as an approximation to the zero of f

The zero of f is

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Thus starting with x_0 (an approximation to the root) pass to a new point x_1 obtained from above. The process can be repeated (iterated) to produce a sequence of points

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

$$x_3 = x_2 - \frac{f(x_2)}{f'(x_2)}$$

The sequence of points will approach a zero (a root) of f say r .

If Newton's method is described in terms of a sequence x_0, x_1, x_2, \dots then the following recursive or inductive definition applies

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Since

$$f'(x_n) = \frac{\Delta y}{\Delta x} = \frac{f(x_n) - 0}{x_n - (x_{n+1})}$$



ACTIVITIES

If $f(x) = x^3 - x + 1$ and $x_0 = 1$

$f(1) = 1$, then $f'(x) = 3x^2 - 1, f'(1) = 2$

$$x_1 = 1 - \frac{1}{2} = \frac{1}{2}$$

$$f\left(\frac{1}{2}\right) = \frac{5}{8}, \quad f'\left(\frac{1}{2}\right) = -\frac{1}{4}$$

$$x_2 = \frac{1}{2} - \frac{\frac{5}{8}x(-4)}{2} = 3$$

$$x_3 = 3 - \frac{25}{26} = 2.0385$$



ACTIVITIES

Use Newton Raphason method to find the square root of 612

Solution

The function to use for $x^2 = 612$ is $f(x) = x^2 - 612 = 0$

$$f'(x) = 2x$$

With an initial guess x_0 of 10

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 10 - \frac{10^2 - 612}{2 \cdot 10} = 35.6$$

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 35.6 - \frac{35.6^2 - 612}{2 \cdot 35.6} = 26.3955056$$

Successive iterations give

$$x_3 = 24.7906355$$

$$x_4 = 24.7386883$$

$$x_5 = 24.7386338$$

Comparing with $\sqrt{612} = 24.73863375$ x_5 is accurate correct to 1×10^{-4}

**ACTIVITIES**

Find the positive root of $f(x) = \cos x - x^3$ using Newton – Raphson's method.

perform four iteration and $x_0 = 0.5$

Solution:

$$f'(x) = -\sin x - 3x^2$$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 0.5 - \frac{-\cos(0.5) - (0.5)^3}{-\sin(0.5) - 3(0.5)^2}$$

$$= 1.1121416 = 1.112$$

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 0.90967 = 0.910$$

$$x_3 = 0.86763 = 0.867 \text{ (3dp)}$$

$$x_4 = 0.865477 = 0.865$$



SELF-TEST QUESTIONS

Exercise

1. Derive the Newton-Raphson iterative formula for solving $f(x) = 0$.
2. Apply Newton-Raphson method to determine a root of the equation
 - i) $f(x) = \cos x - x e^x = 0, \quad x_0 = 0$
 - ii) $f(x) = x^3 + 2x^2 + 10x - 20, \quad x_0 = 1.0$
 - iii) $f(x) = 2x^3 - 5x^2 - 3, \quad x_0 = 2.0$
3. Locate the root of $f(x) = e^{-x} - x$ that is nearest to $\frac{\pi}{2}$
4. Use Newton-Raphson method to find a solution accurate to within 10^{-4} for the given function on the indicated interval
 - i) $x^3 - 2x^2 - 5 = 0, \quad [1, 4]$
 - ii) $x^3 + 3x^2 - 1 = 0, \quad [-3, -2]$
 - iii) $x - \cos x \quad [0, \frac{\pi}{2}]$

6.7. The Δ^2 process (Aitken's Δ^2 method)

This process applies the idea of extrapolation to the limit in order to accelerate convergence.

Let r be the root of the function $f(x) = 0$ and e_n the error in the n^{th} iteration, then

$$e_n = r - x_n = F(r) - F(x_{n-1})$$

$$= F'(\xi)(r - x_{n-1}) = F'(\xi)E_{N-1}$$

$$r - x_{n+1} \simeq F'(r)(r - x_n)$$

$$r - x_{n+2} \simeq F'(r)(r - x_{n+1})$$

Dividing

$$\frac{r - x_{n+1}}{r - x_{n+2}} = \frac{r - x_n}{r - x_{n+1}}$$

Solving for the root r we obtain

$$r = x_{n+2} - \frac{(x_{n+2} - x_{n+1})^2}{x_{n+2} - 2x_{n+1} + x_n}$$

$$r = x_{n+2} - \frac{(\Delta x_{n+1})^2}{\Delta^2 x_n} \text{-----} (*)$$

(Δ is the forward difference)

Equation -----(*) above is the approximation formula for Aithen's method.

x_n is obtained by writing $x = F(x)$ and $x_n = F(x_{n-1})$. For example $x_1 = F(x_0)$, $x_2 = F(x_1)$. once x_0 (initial approximation) x_1 and x_2 are known the rest can be obtained

For example

$$x_3 = x_2 - \frac{(x_2 - x_1)^2}{x_2 - 2x_1 + x_0}$$

$$x_4 = F(x_3), x_5 = F(x_4)$$

$$x_6 = x_5 - \frac{(x_5 - x_4)^2}{x_5 - 2x_4 + x_3}$$

$$x_7 = F(x_6), x_8 = F(x_7)$$

$$x_9 = x_8 - \frac{x_8 - x_7}{x_8 - 2x_7 + x_6}$$



ACTIVITIES

Solve $x^3 + 2x^2 + 10x - 20 = 0$ using Aitken's Δ^2 method

solution

$$\text{Let } x_0 = 1, x(x^2 + 2x + 10) = 20$$

$$x = F(x) = \frac{20}{x^2 + 2x + 10}$$

$$x_1 = F(x_0) = F(1) = \frac{20}{13} = 1.538461538$$

$$x_2 = F(x_1) = \frac{20}{\left(\frac{20}{13}\right)^2 + 2\left(\frac{20}{13}\right) + 10} = 1.295019157$$

$$x_3 = x_2 - \frac{(x_2 - x_1)^2}{x_2 - 2x_1 + x_0} = 1.370813882$$

$$x_4 = F(x_3), x_5 = F(x_4)$$

$$x_6 = x_5 - \frac{(x_5 - x_4)^2}{x_5 - 2x_4 + x_3} = 1.368808169$$

$$x_7 = F(x_6), x_8 = F(x_7)$$

$$x_9 = x_8 - \frac{(x_8 - x_7)^2}{x_8 - 2x_7 + x_6} = 1.368808108$$

and so on

The equation

$x^3 + 2x^2 + 10x - 20 = 0$, is commonly known as Leonardo's equation and

its exact solution is 1.368808107



SELF-TEST QUESTIONS

Solve the following equations using Aitken's Δ^2 method

i) $x^3 + 4x^2 - 10 = 0$

ii) $2x^3 - 5x^2 - 3 = 0$

iii) $x^3 - 2x^3 - 5 = 0$



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1. **Numerical Analysis: Richard L. Burden, J. Douglas Faires**
2. **Numerical Methods for Scientific and Engineering Computation: M. K. Jain**
3. **Numerical Analysis: Schaum's Outline Series**
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