Solution of Nonlinear Equations

Solution of Nonlinear Equations

(Root Finding Problems)

- Definitions
- Classification of Methods
  - Analytical Solutions
  - Graphical Methods
  - Numerical Methods
    - Bracketing Methods
    - Open Methods
- Convergence Notations

Root Finding Problems

Many problems in Science and Engineering are expressed as:

$$\boxed{\begin{array}{l}\text{Given a continuous function } f(x), \\ \text{find the value } r \text{ such that } f(r) = 0\end{array}}$$

These problems are called root finding problems.

Roots of Equations

A number *r* that satisfies an equation is called a root of the equation.

The equation: $x^4 - 3x^3 - 7x^2 + 15x = -18$

has four roots: $-2,\ 3,\ 3,\ and\ -1$.

i.e., $x^4 - 3x^3 - 7x^2 + 15x + 18 = (x+2)(x-3)^2(x+1)$

The equation has two simple roots $(-1$ and $-2)$

and a repeated root (3) with multiplicity $= 2$.

Zeros of a Function

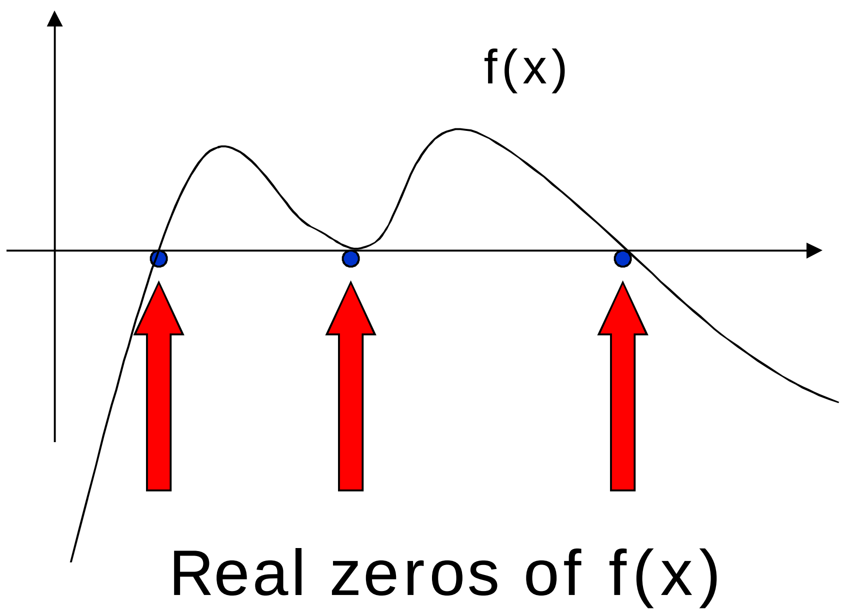
Let $f(x)$ be a real-valued function of a real variable. Any number r for which $f(r)=0$ is called a zero of the function.

Examples:

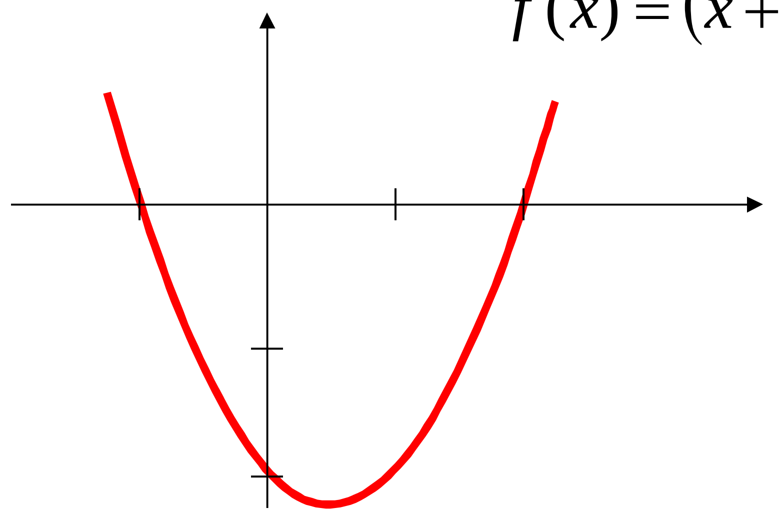
2 and 3 are zeros of the function $f(x) = (x-2)(x-3)$.

Graphical Interpretation of Zeros

- The real zeros of a function ***f(x)*** are the values of ***x*** at which the graph of the function crosses (or touches) the x-axis.



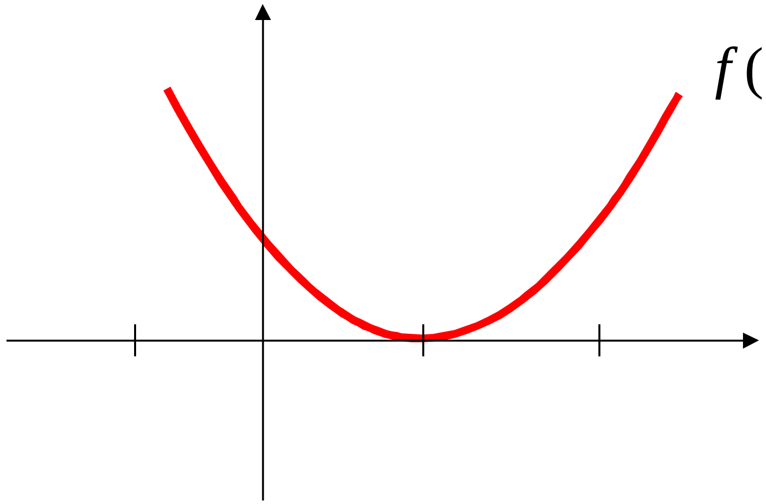
Simple Zeros



$$f(x) = (x+1)(x-2) = x^2 - x - 2$$

has two simple zeros (one at x = 2 and one at x = –1)

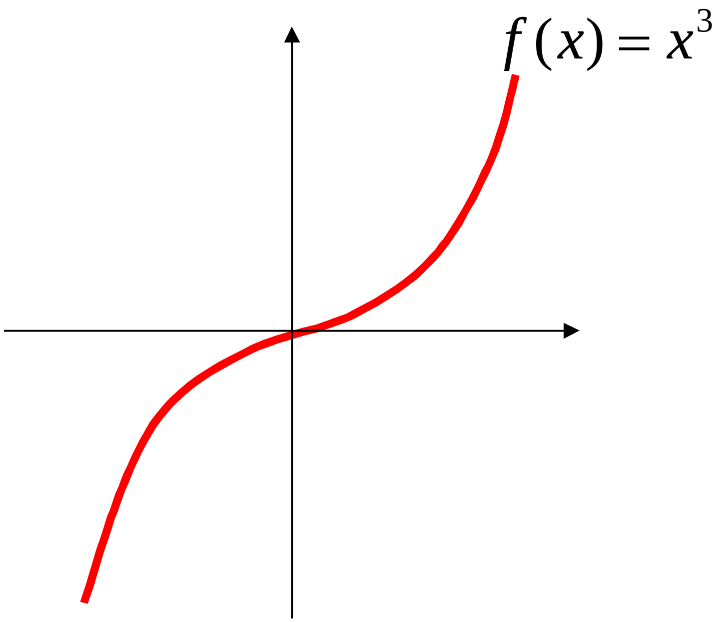
Multiple Zeros



$$f(x) = (x-1)^2 = x^2 - 2x + 1$$

has double zeros (zero with muliplicity = 2) at x = 1

Multiple Zeros



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

has a zero with muliplicity $= 3$ at $\mathrm{x} = 0$

Facts

- Any n^{th} order polynomial has exactly n zeros (counting real and complex zeros with their multiplicities).
- Any polynomial with an odd order has at least one real zero.
- If a function has a zero at $\boldsymbol{x=r}$ with multiplicity $\boldsymbol{m}$ then the function and its first $\boldsymbol{(m-1)}$ derivatives are zero at $\boldsymbol{x=r}$ *and the* $\boldsymbol{m}^{th}$ *derivative at* $\boldsymbol{r}$ *is not zero*.

Roots of Equations & Zeros of Function

Given the equation:

$$x^4 - 3x^3 - 7x^2 + 15x = -18$$

Move all terms to one side of the equation:

$$x^4 - 3x^3 - 7x^2 + 15x + 18 = 0$$

Define $f(x)$ as:

$$f(x) = x^4 - 3x^3 - 7x^2 + 15x + 18$$

The zeros of $f(x)$ are the same as the roots of the equation $f(x) = 0$

(Which are -2, 3, 3, and -1)

Solution Methods

Several ways to solve nonlinear equations are possible:

- Analytical Solutions
  - Possible for special equations only
- Graphical Solutions
  - Useful for providing initial guesses for other methods
- Numerical Solutions
  - Open methods
  - Bracketing methods

Analytical Methods

Analytical Solutions are available for special equations only.

$$\text{Analytical solution of}: \; a\,x^2 + b\,x + c = 0$$

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

$$\text{No analytical solution is available for}: \quad x - e^{-x} = 0$$

Graphical Methods

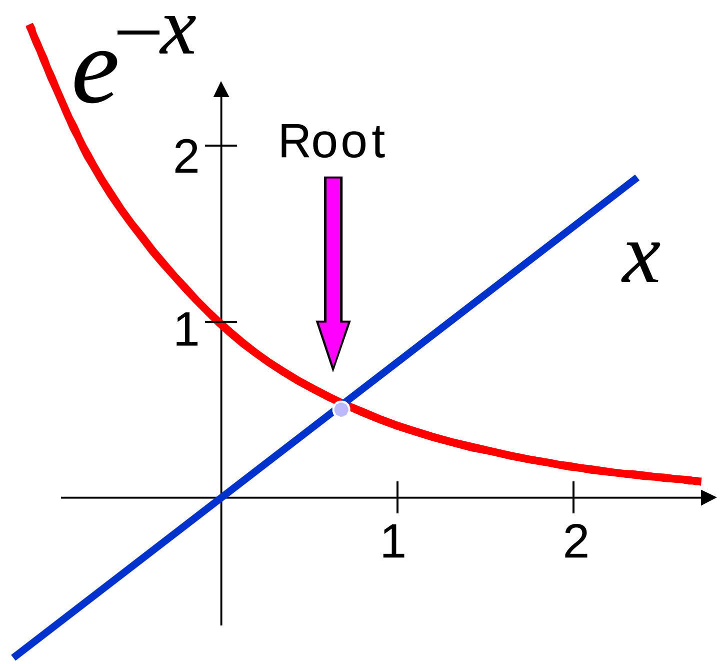
- Graphical methods are useful to provide an initial guess to be used by other methods.

$$Solve$$

$$x = e^{-x}$$

$$The \;\; root \in [0,1]$$

$$root \approx 0.6$$



Numerical Methods

Many methods are available to solve nonlinear equations:

- Bisection Method
- Newton's Method
- Secant Method

These will be covered in CISE301

- False position Method
- Muller's Method
- Bairstow's Method
- Fixed point iterations
- ……….

Bracketing Methods

- In bracketing methods, the method starts with an interval that contains the root and a procedure is used to obtain a smaller interval containing the root.

- Examples of bracketing methods:
  - Bisection method
  - False position method

Open Methods

- In the open methods, the method starts with one or more initial guess points. In each iteration, a new guess of the root is obtained.
- Open methods are usually more efficient than bracketing methods.
- They may not converge to a root.

Convergence Notation

A sequence $x_1, x_2, \ldots, x_n, \ldots$ is said to **converge** to x if to every $\varepsilon > 0$ there exists N such that:

$$\left| x_n - x \right| < \varepsilon \quad \forall n > N$$

Convergence Notation

Let $x_1, x_2, \ldots.,$ converge to $x.$

Linear Convergence : $$\frac{|x_{n+1}-x|}{|x_n-x|} \le C$$

Quadratic Convergence : $$\frac{|x_{n+1}-x|}{|x_n-x|^2} \le C$$

Convergence of order P : $$\frac{|x_{n+1}-x|}{|x_n-x|^p} \le C$$

Speed of Convergence

- We can compare different methods in terms of their convergence rate.
- Quadratic convergence is faster than linear convergence.
- A method with convergence order q converges faster than a method with convergence order p if $q > p$.
- Methods of convergence order $p > 1$ are said to have super linear convergence.

Lectures 6-7

Bisection Method

- The Bisection Algorithm
- Convergence Analysis of Bisection Method
- Examples

Reading Assignment: Sections 5.1 and 5.2

Introduction

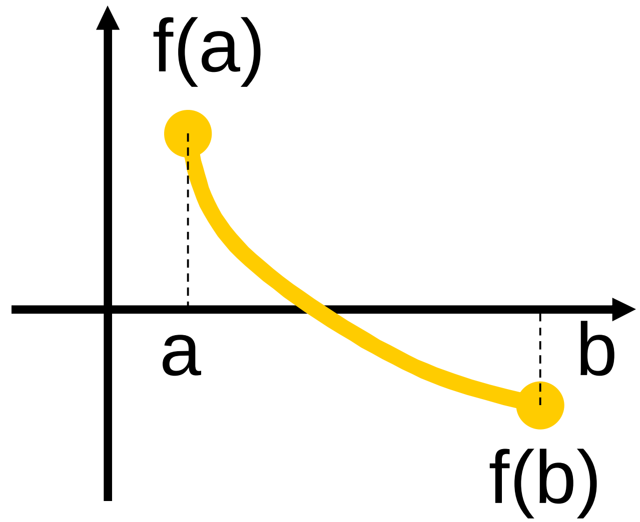
- The **Bisection method** is one of the simplest methods to find a zero of a nonlinear function.
- It is also called **interval halving** method.
- To use the Bisection method, one needs an initial interval that is known to contain a zero of the function.
- The method systematically reduces the interval. It does this by dividing the interval into two equal parts, performs a simple test and based on the result of the test, half of the interval is thrown away.
- The procedure is repeated until the desired interval size is obtained.

Intermediate Value Theorem

- Let f(x) be defined on the interval [a,b].

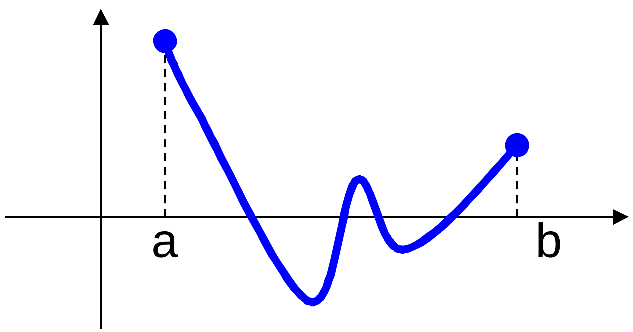
- Intermediate value theorem:

  if a function is continuous and f(a) and f(b) have different signs then the function has at least one zero in the interval [a,b].

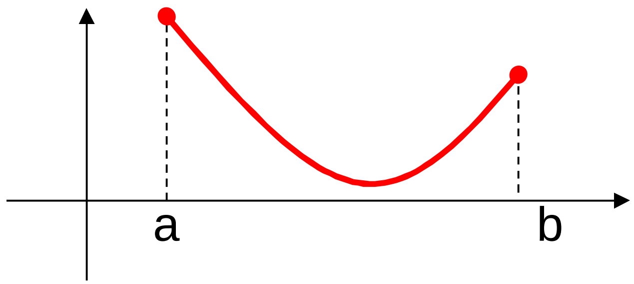


Examples

- If f(a) and f(b) have the same sign, the function may have an even number of real zeros or no real zeros in the interval [a, b].
- Bisection method can not be used in these cases.



The function has four real zeros

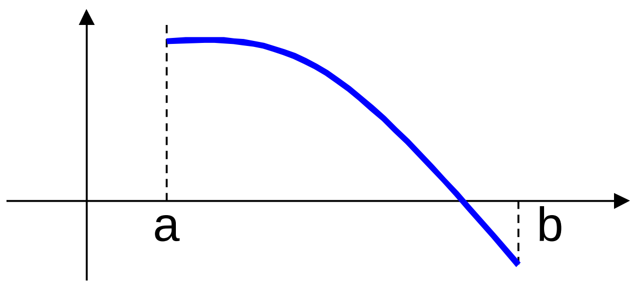


The function has no real zeros

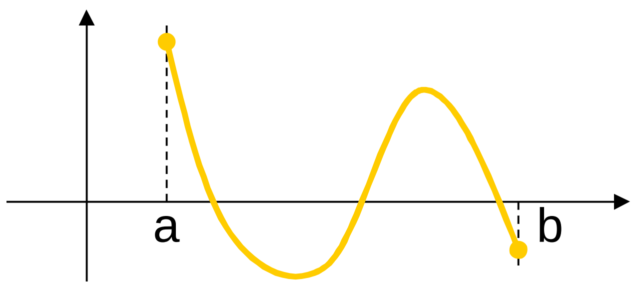
Two More Examples

- If f(a) and f(b) have different signs, the function has at least one real zero.

- Bisection method can be used to find one of the zeros.



The function has one real zero



The function has three real zeros

Bisection Method

- If the function is continuous on [a,b] and f(a) and f(b) have different signs, Bisection method obtains a new interval that is half of the current interval and the sign of the function at the end points of the interval are different.

- This allows us to repeat the Bisection procedure to further reduce the size of the interval.

Bisection Method

Assumptions:

Given an interval [a,b]

f(x) is continuous on [a,b]

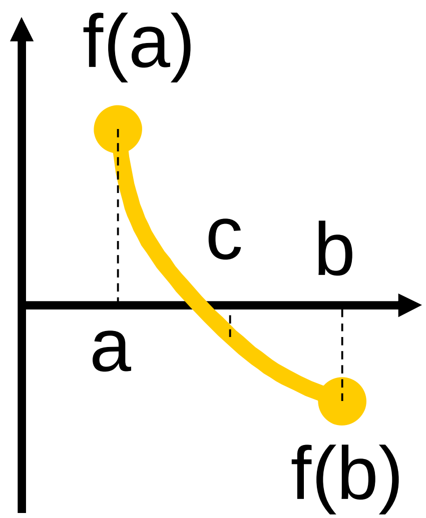
f(a) and f(b) have opposite signs.

These assumptions ensure the existence of at least one zero in the interval [a,b] and the bisection method can be used to obtain a smaller interval that contains the zero.

Bisection Algorithm

Assumptions:

- f(x) is continuous on [a,b]
- f(a) f(b) < 0



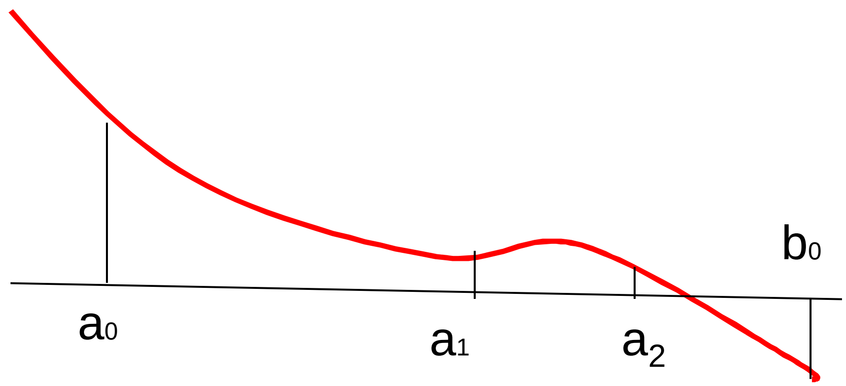
Algorithm:

Loop

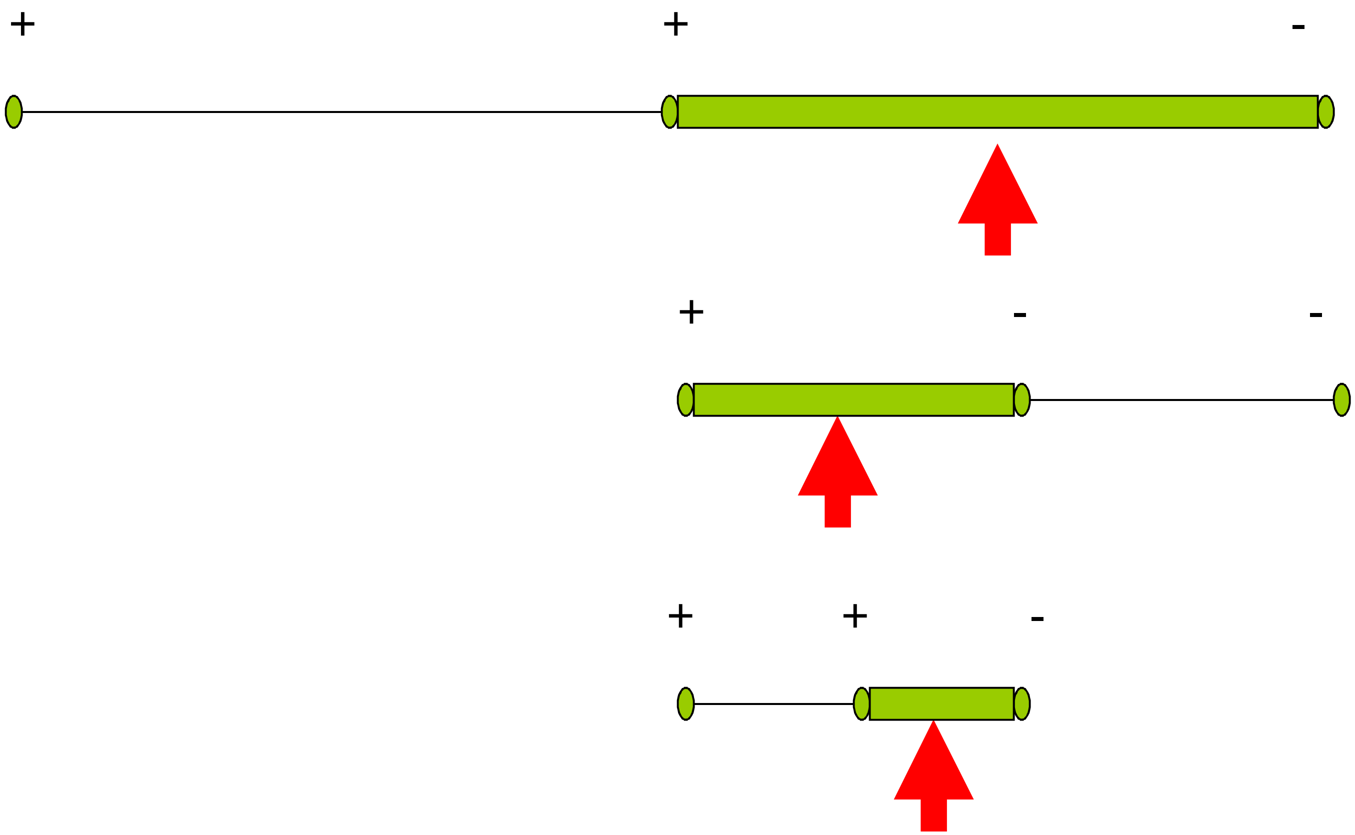
1. Compute the mid point c=(a+b)/2
2. Evaluate f(c)
3. If f(a) f(c) < 0 then new interval [a, c]
   If f(a) f(c) > 0 then new interval [c, b]

End loop

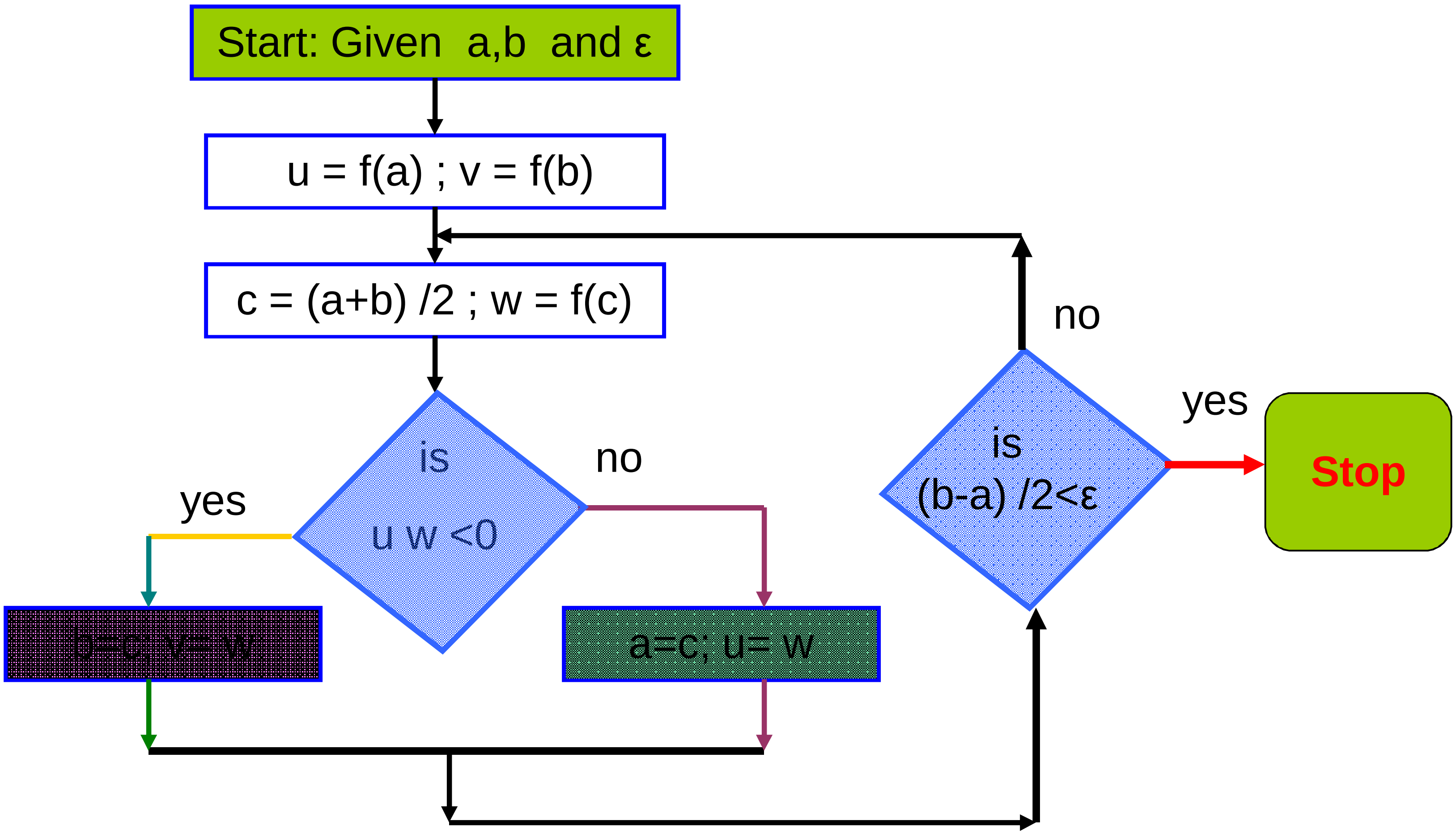
Bisection Method



Example



Flow Chart of Bisection Method



Example

Can you use Bisection method to find a zero of :

$f(x) = x^3 - 3x + 1$ in the interval [0,2]?

Answer:

$f(x)$ is continuous on $[0,2]$

and $f(0) * f(2) = (1)(3) = 3 > 0$

$\Rightarrow$ Assumptions are not satisfied

$\Rightarrow$ Bisection method can not be used

Example

Can you use Bisection method to find a zero of :

$f(x) = x^3 - 3x + 1$ in the interval $[0,1]$?

Answer:

$f(x)$ is continuous on $[0,1]$

and $f(0) * f(1) = (1)(-1) = -1 < 0$

$\Rightarrow$ Assumptions are satisfied

$\Rightarrow$ Bisection method can be used

Best Estimate and Error Level

Bisection method obtains an interval that is guaranteed to contain a zero of the function.

Questions:

- What is the best estimate of the zero of ***f(x)***?
- What is the error level in the obtained estimate?

Best Estimate and Error Level

The best estimate of the zero of the function ***f(x)*** after the first iteration of the Bisection method is the mid point of the initial interval:

$$Estimate\ of\ the\ zero:\ \ r = \frac{b+a}{2}$$

$$Error \leq \frac{b-a}{2}$$

Stopping Criteria

Two common stopping criteria

1. Stop after a fixed number of iterations
2. Stop when the absolute error is less than a specified value

How are these criteria related?

Stopping Criteria

c_n : is the midpoint of the interval at the n[th] iteration

(c_n is usually used as the estimate of the root).

r : is the zero of the function.

After n iterations :

$$\left| error \right| = \left| r - c_n \right| \leq E_a^n = \frac{b-a}{2^n} = \frac{\Delta x^0}{2^n}$$

Convergence Analysis

Given $f(x), a, b, and \ \varepsilon$

How many iterations are needed such that: $|x - r| \le \varepsilon$

where r is the zero of *f(x)* and x is the

bisection estimate (i.e., $x = c_k$)?

$$n \ge \frac{\log(b-a) - \log(\varepsilon)}{\log(2)}$$

Convergence Analysis – Alternative Form

$$n \geq \frac{\log(b-a) - \log(\varepsilon)}{\log(2)}$$

$$n \geq \log_2\left(\frac{\text{width of initial interval}}{\text{desired error}}\right) = \log_2\left(\frac{b-a}{\varepsilon}\right)$$

Example

$$a = 6, \;\; b = 7, \; \varepsilon = 0.0005$$

How many iterations are needed such that : $\left| x - r \right| \leq \varepsilon$?

$$n \geq \frac{\log(b-a) - \log(\varepsilon)}{\log(2)} = \frac{\log(1) - \log(0.0005)}{\log(2)} = 10.9658$$

$$\Rightarrow n \geq 11$$

Example

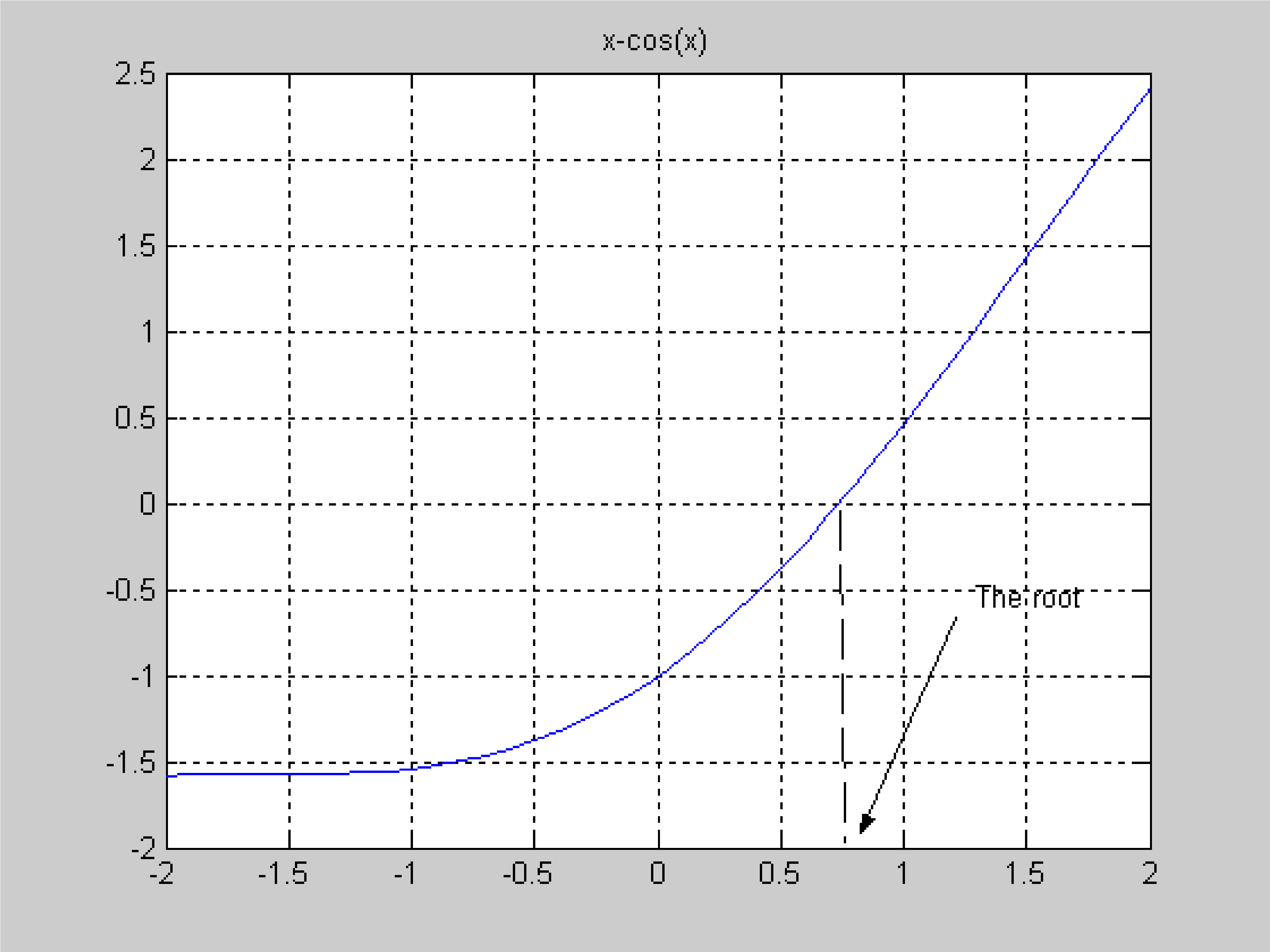
- Use Bisection method to find a root of the equation $x = \cos(x)$ with absolute error <0.02
  (assume the initial interval [0.5, 0.9])

Question 1: What is $f(x)$?

Question 2: Are the assumptions satisfied ?

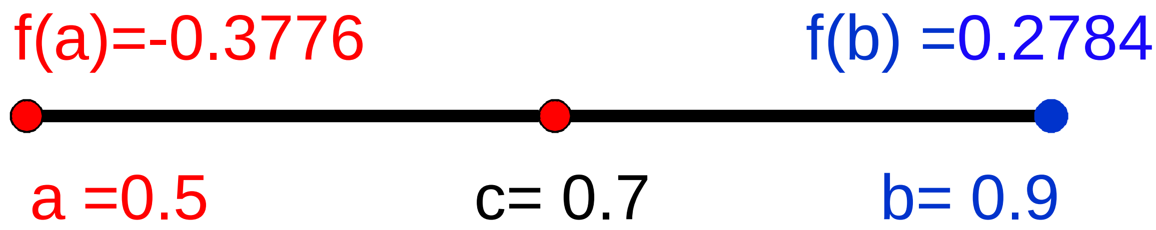
Question 3: How many iterations are needed ?

Question 4: How to compute the new estimate ?


x-cos(x)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
The root

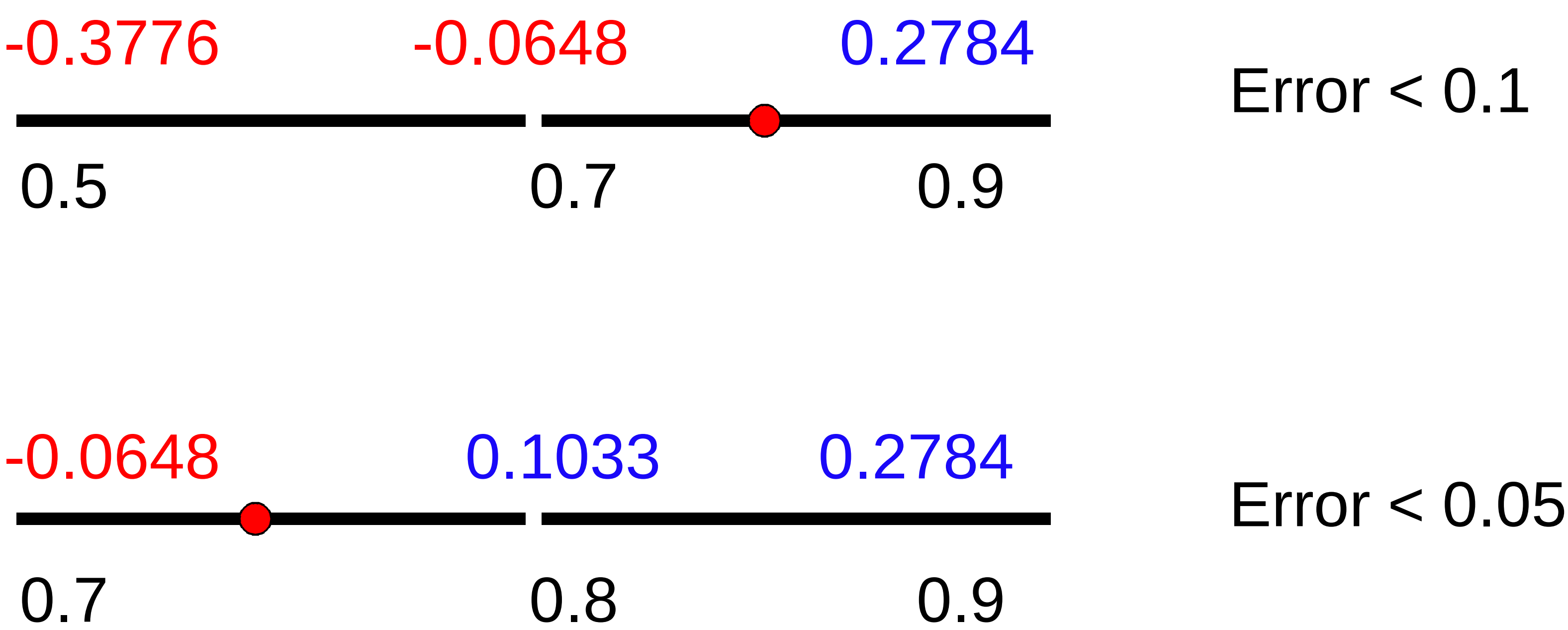
Bisection Method

Initial Interval

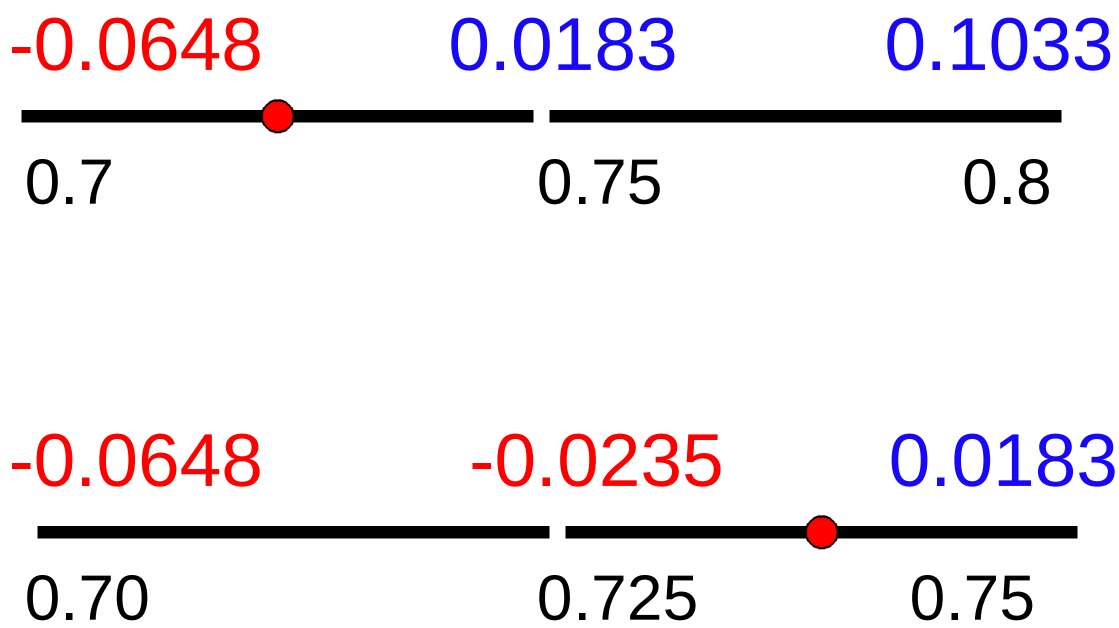


Error < 0.2

Bisection Method



Bisection Method



Error < 0.025

Error < .0125

Summary

- Initial interval containing the root: [0.5,0.9]

- After 5 iterations:
  - Interval containing the root: [0.725, 0.75]
  - Best estimate of the root is 0.7375
  - $|\text{ Error }| < 0.0125$

A Matlab Program of Bisection Method

```
a=.5; b=.9;
u=a-cos(a);
v=b-cos(b);
    for i=1:5
        c=(a+b)/2
        fc=c-cos(c)
        if u*fc<0
          b=c ; v=fc;
        else
          a=c; u=fc;
        end
    end
```

```
c =
   0.7000
fc =
  -0.0648
c =
   0.8000
fc =
   0.1033
c =
   0.7500
fc =
   0.0183
c =
   0.7250
fc =
  -0.0235
```

Example

Find the root of:

$$f(x) = x^3 - 3x + 1 \text{ in the interval:}[0,1]$$

* $f(x)$ is continuous

* $f(0) = 1, \; f(1) = -1 \Rightarrow f(a)\, f(b) < 0$

$\Rightarrow$ Bisection method can be used to find the root

Example

Iteration	a	b	c= $\frac{(a+b)}{2}$	f(c)	$\frac{(b-a)}{2}$
1	0	1	0.5	-0.375	0.5
2	0	0.5	0.25	0.266	0.25
3	0.25	0.5	.375	-7.23E-3	0.125
4	0.25	0.375	0.3125	9.30E-2	0.0625
5	0.3125	0.375	0.34375	9.37E-3	0.03125

Bisection Method

Advantages

- Simple and easy to implement
- One function evaluation per iteration
- The size of the interval containing the zero is reduced by 50% after each iteration
- The number of iterations can be determined a priori
- No knowledge of the derivative is needed
- The function does not have to be differentiable

Disadvantage

- Slow to converge
- Good intermediate approximations may be discarded

Lecture 8-9
Newton-Raphson Method

- Assumptions
- Interpretation
- Examples
- Convergence Analysis

Newton-Raphson Method

(Also known as Newton's Method)

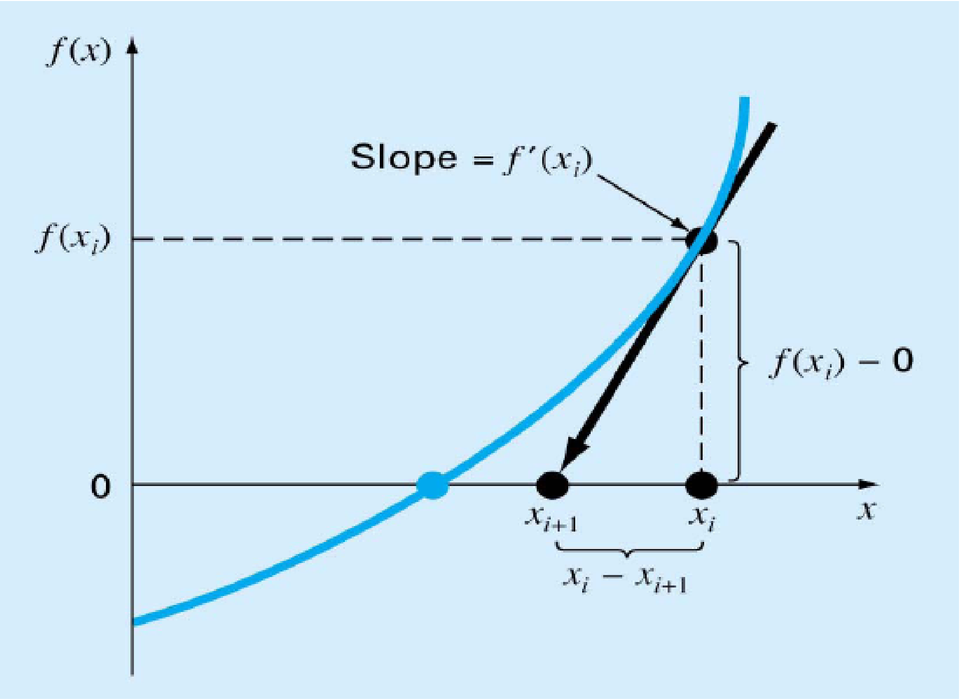
Given an initial guess of the root x_0, Newton-Raphson method uses information about the function and its derivative at that point to find a better guess of the root.

Assumptions:

- $f(x)$ is continuous and the first derivative is known
- An initial guess x_0 such that $f'(x_0) \neq 0$ is given

Newton Raphson Method
- Graphical Depiction -

- If the initial guess at the root is $\boldsymbol{x_i}$, then a tangent to the function of $\boldsymbol{x_i}$ that is $\boldsymbol{f'(x_i)}$ is extrapolated down to the *x-axis* to provide an estimate of the root at $\boldsymbol{x_{i+1}}$.



Derivation of Newton's Method

$\mathit{Given}: x_i$ an initial guess of the root of $f(x) = 0$

$\mathit{Question}$: How do we obtain a better estimate x_{i+1}?

Taylor Therorem : $f(x+h) \approx f(x) + f'(x)h$

Find h such that $f(x+h) = 0$.

$$\Rightarrow h \approx -\frac{f(x)}{f'(x)}$$

Newton – Raphson Formula

A new guess of the root : $x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x_i)}$

Newton's Method

$$Given \quad f(x),\ f'(x),\ x_0$$

$$Assumption \quad f'(x_0) \neq 0$$

$$for \quad i = 0:n$$

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

$$end$$

```
C    FORTRAN  PROGRAM
       F(X) = X**3 - 3*X**2 + 1
       FP(X) = 3*X**2 - 6*X
       X = 4
       DO  10 I = 1,5
        X = X - F(X)/FP(X)
        PRINT *,  X
10      CONTINUE
       STOP
       END
```

Newton's Method

$$Given \quad f(x),\ f'(x),\ x_0$$

$$Assumption \quad f'(x_0) \neq 0$$

$$for \quad i = 0:n$$

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

$$end$$

F.m

$$function \quad [F] = F(X)$$

$$F = X^\wedge 3 - 3 * X^\wedge 2 + 1$$

FP.m

$$function \quad [FP] = FP(X)$$

$$FP = 3 * X^\wedge 2 - 6 * X$$

$$\% \quad MATLAB \ PROGRAM$$

$$X = 4$$

$$for \ i = 1:5$$

$$X = X - F(X)/FP(X)$$

$$end$$

Example

Find a zero of the function $f(x) = x^3 - 2x^2 + x - 3$, $x_0 = 4$

$f'(x) = 3x^2 - 4x + 1$

Iteration 1: $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 4 - \frac{33}{33} = 3$

Iteration 2: $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 3 - \frac{9}{16} = 2.4375$

Iteration 3: $x_3 = x_2 - \frac{f(x_2)}{f'(x_2)} = 2.4375 - \frac{2.0369}{9.0742} = 2.2130$

Example

k (Iteration)	x_k	$f(x_k)$	$f'(x_k)$	x_{k+1}	$\lvert x_{k+1} - x_k \rvert$
0	**4**	**33**	**33**	**3**	1
1	**3**	**9**	**16**	**2.4375**	0.5625
2	**2.4375**	**2.0369**	**9.0742**	**2.2130**	0.2245
3	**2.2130**	**0.2564**	**6.8404**	**2.1756**	0.0384
4	**2.1756**	**0.0065**	**6.4969**	**2.1746**	0.0010

Convergence Analysis

Theorem :

Let $f(x), f'(x)$ *and* $f''(x)$ be continuous at x ≈ r

where $f(r) = 0$. *If* $f'(r) \neq 0$ then there exists $\delta > 0$

such that $|x_0 - r| \le \delta \Rightarrow \dfrac{|x_{k+1} - r|}{|x_k - r|^2} \le C$

$$C = \frac{1}{2} \frac{\max\limits_{|x_0 - r| \le \delta} |f''(x)|}{\min\limits_{|x_0 - r| \le \delta} |f'(x)|}$$

Convergence Analysis
Remarks

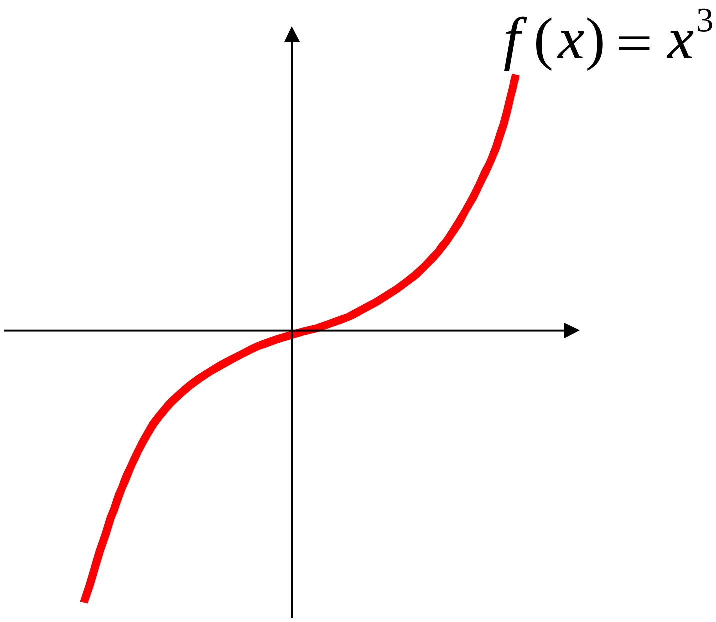
When the guess is close enough to a simple root of the function then Newton's method is guaranteed to converge quadratically.

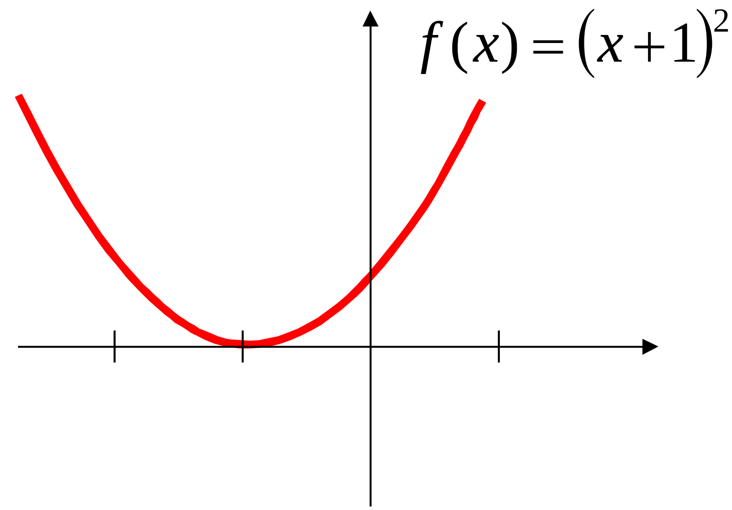
Quadratic convergence means that the number of correct digits is nearly doubled at each iteration.

Problems with Newton's Method

- If the initial guess of the root is far from the root the method may not converge.
- Newton's method converges linearly near multiple zeros { $f(r) = f'(r) = 0$ }. In such a case, modified algorithms can be used to regain the quadratic convergence.

Multiple Roots

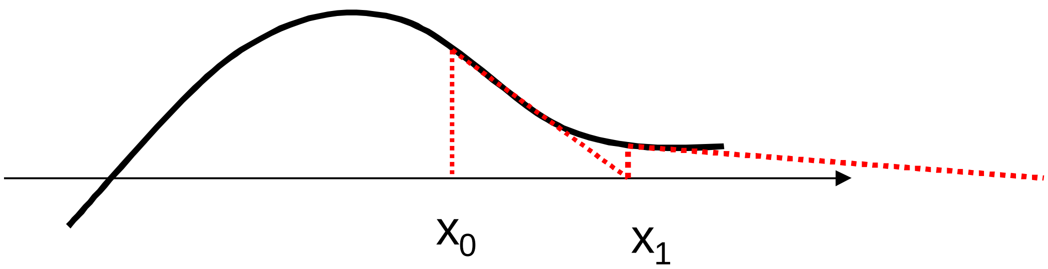




f(x) has three zeros at x = 0

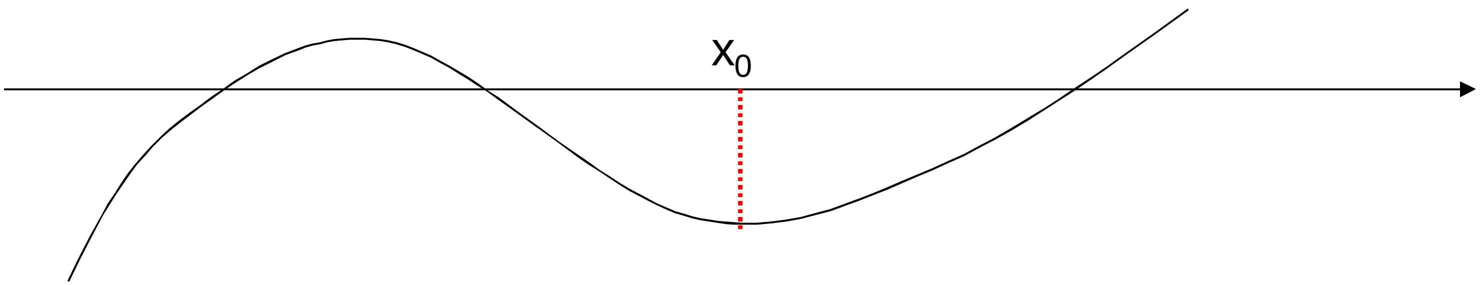
f(x) has two zeros at x = -1

Problems with Newton's Method
- Runaway -



The estimates of the root is going away from the root.

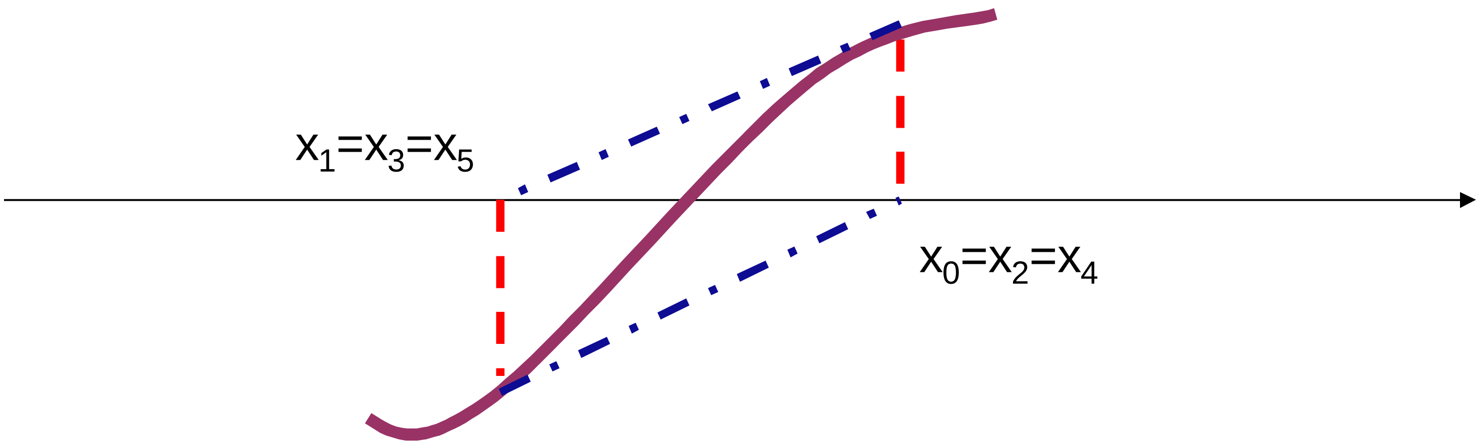
Problems with Newton's Method
- Flat Spot -



The value of ***f'(x)*** is zero, the algorithm fails.

If ***f '(x)*** is very small then $\boldsymbol{x_1}$ will be very far from $\boldsymbol{x_0}$.

Problems with Newton's Method
- Cycle -



The algorithm cycles between two values x_0 and x_1

Newton's Method for Systems of Non Linear Equations

$$Given:\ X_0 \text{ an initial guess of the root of } F(x)=0$$

$$Newton's\ Iteration$$

$$X_{k+1} = X_k - \left[F'(X_k)\right]^{-1} F(X_k)$$

$$F(X)=\begin{bmatrix} f_1(x_1,x_2,\ldots) \\ f_2(x_1,x_2,\ldots) \\ \vdots \end{bmatrix},\quad F'(X)=\begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \dfrac{\partial f_1}{\partial x_2} & \vdots \\ \dfrac{\partial f_2}{\partial x_1} & \dfrac{\partial f_2}{\partial x_2} & \\ \vdots & & \end{bmatrix}$$

Example

- Solve the following system of equations:

$$y + x^2 - 0.5 - x = 0$$

$$x^2 - 5xy - y = 0$$

$$\text{Initial guess } \; x = 1, \;\; y = 0$$

$$F = \begin{bmatrix} y + x^2 - 0.5 - x \\ x^2 - 5xy - y \end{bmatrix}, \; F' = \begin{bmatrix} 2x - 1 & 1 \\ 2x - 5y & -5x - 1 \end{bmatrix}, X_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Solution Using Newton's Method

Iteration 1:

$$F=\begin{bmatrix} y+x^2-0.5-x \\ x^2-5xy-y \end{bmatrix}=\begin{bmatrix} -0.5 \\ 1 \end{bmatrix}=,\quad F'=\begin{bmatrix} 2x-1 & 1 \\ 2x-5y & -5x-1 \end{bmatrix}=\begin{bmatrix} 1 & 1 \\ 2 & -6 \end{bmatrix}$$

$$X_1=\begin{bmatrix} 1 \\ 0 \end{bmatrix}-\begin{bmatrix} 1 & 1 \\ 2 & -6 \end{bmatrix}^{-1}\begin{bmatrix} -0.5 \\ 1 \end{bmatrix}=\begin{bmatrix} 1.25 \\ 0.25 \end{bmatrix}$$

Iteration 2:

$$F=\begin{bmatrix} 0.0625 \\ -0.25 \end{bmatrix}=,\quad F'=\begin{bmatrix} 1.5 & 1 \\ 1.25 & -7.25 \end{bmatrix}$$

$$X_2=\begin{bmatrix} 1.25 \\ 0.25 \end{bmatrix}-\begin{bmatrix} 1.5 & 1 \\ 1.25 & -7.25 \end{bmatrix}^{-1}\begin{bmatrix} 0.0625 \\ -0.25 \end{bmatrix}=\begin{bmatrix} 1.2332 \\ 0.2126 \end{bmatrix}$$

Example

Try this

- Solve the following system of equations:

$$y + x^2 - 1 - x = 0$$

$$x^2 - 2y^2 - y = 0$$

$$\text{Initial guess } x = 0, \quad y = 0$$

$$F = \begin{bmatrix} y + x^2 - 1 - x \\ x^2 - 2y^2 - y \end{bmatrix}, \quad F' = \begin{bmatrix} 2x - 1 & 1 \\ 2x & -4y - 1 \end{bmatrix}, \quad X_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Example

Solution

$Iteration$	0	1	2	3	4	5
X_k	$\begin{bmatrix} 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -1 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -0.6 \\ 0.2 \end{bmatrix}$	$\begin{bmatrix} -0.5287 \\ 0.1969 \end{bmatrix}$	$\begin{bmatrix} -0.5257 \\ 0.1980 \end{bmatrix}$	$\begin{bmatrix} -0.5257 \\ 0.1980 \end{bmatrix}$

Lectures 10

Secant Method

- Secant Method
- Examples
- Convergence Analysis

Newton's Method (Review)

$$Assumptions: \quad f(x),\ f'(x),\ x_0 \quad are\ available,$$

$$f'(x_0) \neq 0$$

$$Newton's\ \ Method\ \ new\ estimate:$$

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Problem:

$f'(x_i)$ is not available,

or difficult to obtain analytically.

Secant Method

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

$$\text{if} \quad x_i \;\; and \;\; x_{i-1} \text{ are two initial points:}$$

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{(x_i - x_{i-1})}$$

$$\boxed{x_{i+1} = x_i - \frac{f(x_i)}{\dfrac{f(x_i) - f(x_{i-1})}{(x_i - x_{i-1})}} = \quad x_i - f(x_i)\frac{(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}}$$

Secant Method

Assumptions:

Two initial points x_i *and* x_{i-1}

such that $f(x_i) \neq f(x_{i-1})$

New estimate (Secant Method):

$$x_{i+1} = x_i - f(x_i)\frac{(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

Secant Method

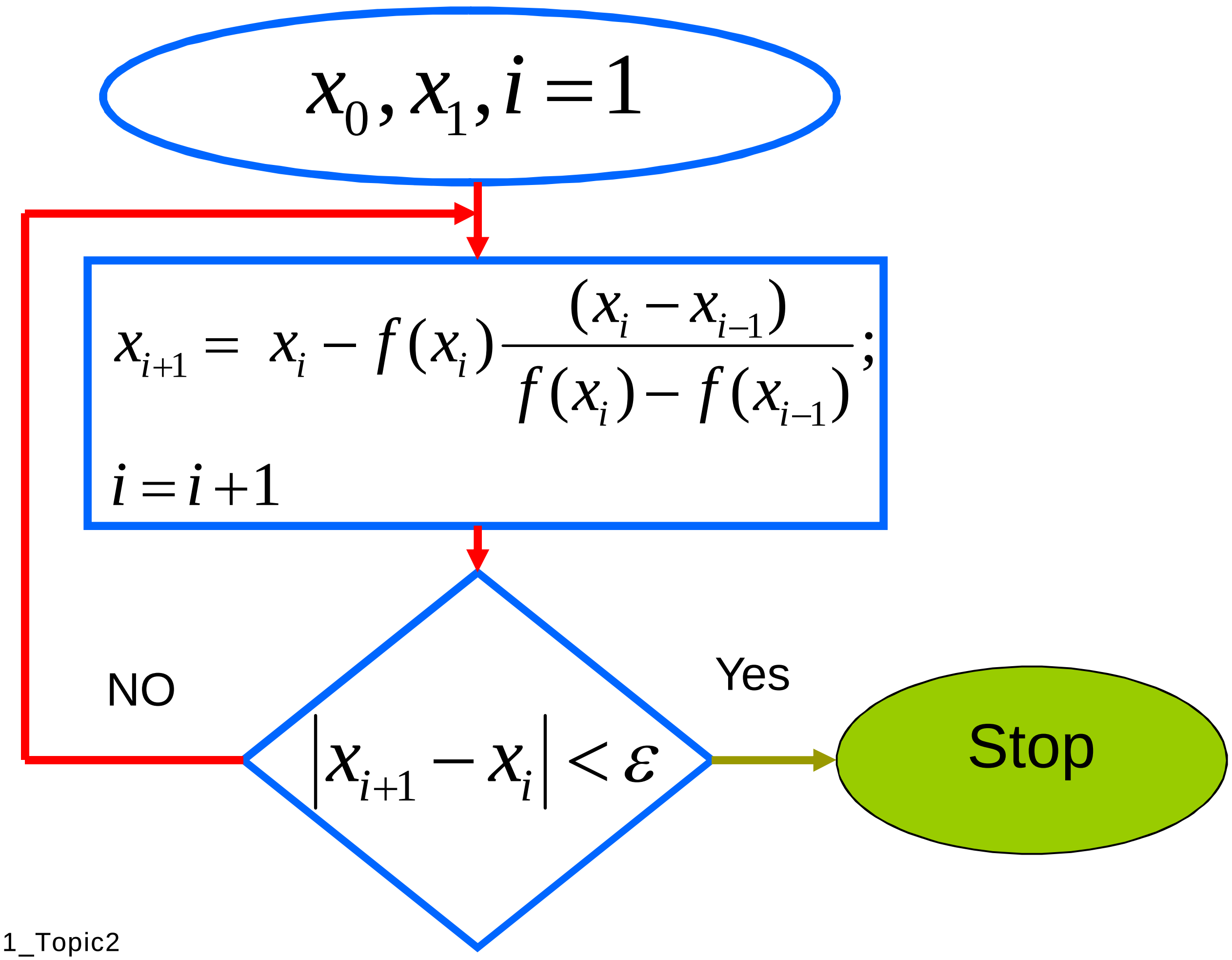
$$f(x) = x^2 - 2x + 0.5$$

$$x_0 = 0$$

$$x_1 = 1$$

$$x_{i+1} = x_i - f(x_i)\frac{(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

Secant Method - Flowchart



Modified Secant Method

In this modified Secant method, only one initial guess is needed :

$$f'(x_i) \approx \frac{f(x_i + \delta x_i) - f(x_i)}{\delta x_i}$$

$$x_{i+1} = x_i - \frac{f(x_i)}{\dfrac{f(x_i + \delta\ x_i) - f(x_i)}{\delta\ x_i}} = \quad x_i - \frac{\delta\, x_i\, f(x_i)}{f(x_i + \delta\ x_i) - f(x_i)}$$

Problem : How to select δ ?

If not selected properly, the method may diverge.

Example

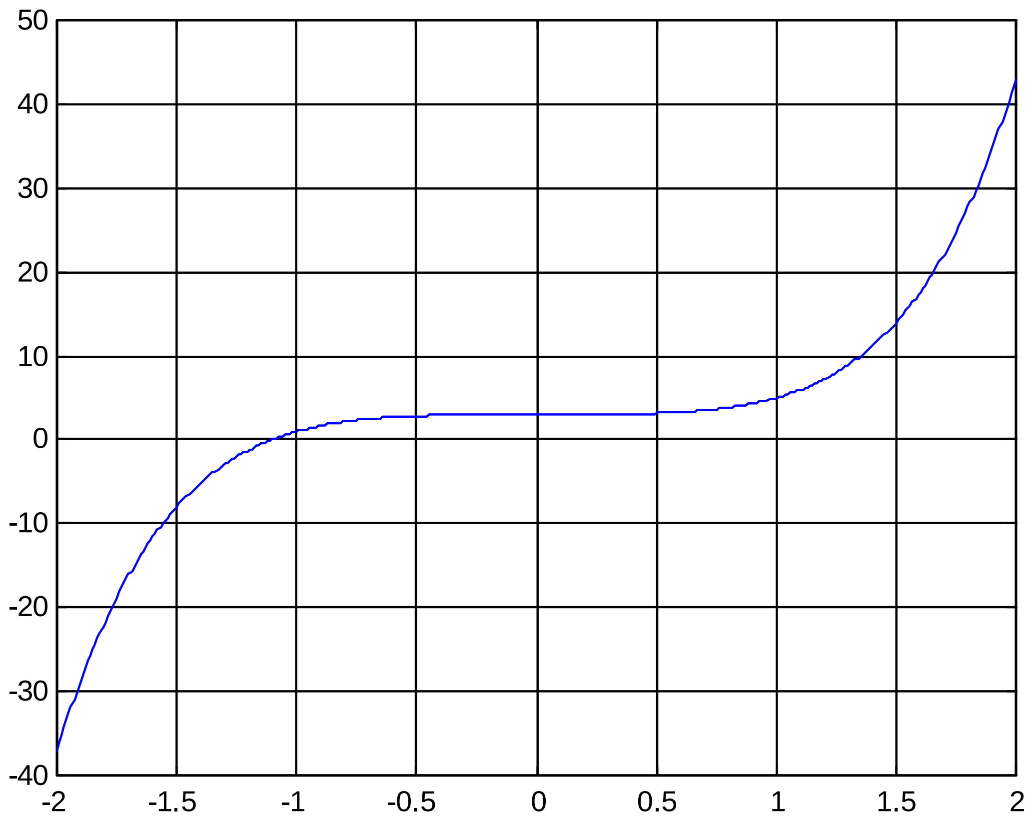
Find the roots of :

$$f(x) = x^5 + x^3 + 3$$

Initial points

$$x_0 = -1 \; and \; x_1 = -1.1$$

$$with \;\; error < 0.001$$



Example

x(i)	f(x(i))	x(i+1)	|x(i+1)-x(i)|
-1.0000	1.0000	-1.1000	0.1000
-1.1000	0.0585	-1.1062	0. 0062
-1.1062	0.0102	-1.1052	0.0009
-1.1052	0.0001	-1.1052	0.0000

Convergence Analysis

- The rate of convergence of the Secant method is super linear:

$$\frac{|x_{i+1}-r|}{|x_i-r|^{\alpha}} \le C, \qquad \alpha \approx 1.62$$

$$r : root \qquad x_i : \text{estimate of the root at the i}^{\text{th}} \text{ iteration.}$$

- It is better than Bisection method but not as good as Newton's method.

Lectures 11

Comparison of Root Finding Methods

- Advantages/disadvantages
- Examples

Summary

Method	Pros	Cons
Bisection	- Easy, Reliable, Convergent - One function evaluation per iteration - No knowledge of derivative is needed	- Slow - Needs an interval [a,b] containing the root, i.e., $f(a)f(b)<0$
Newton	- Fast (if near the root) - Two function evaluations per iteration	- May diverge - Needs derivative and an initial guess x_0 such that $f'(x_0)$ is nonzero
Secant	- Fast (slower than Newton) - One function evaluation per iteration - No knowledge of derivative is needed	- May diverge - Needs two initial points guess x_0, x_1 such that $f(x_0)- f(x_1)$ is nonzero

Example

Use Secant method to find the root of :

$f(x) = x^6 - x - 1$

Two initial points $x_0 = 1$ *and* $x_1 = 1.5$

$$x_{i+1} = x_i - f(x_i)\frac{(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

Solution

k	x_k	$f(x_k)$
0	1.0000	-1.0000
1	1.5000	8.8906
2	1.0506	-0.7062
3	1.0836	-0.4645
4	1.1472	0.1321
5	1.1331	-0.0165
6	1.1347	-0.0005

Example

Use Newton's Method to find a root of :

$$f(x) = x^3 - x - 1$$

Use the initial point : $x_0 = 1$.

Stop after three iterations, or

if $\left| x_{k+1} - x_k \right| < 0.001$, or

if $\left| f(x_k) \right| < 0.0001$.

Five Iterations of the Solution

k	x_k	$f(x_k)$	$f'(x_k)$	ERROR
0	1.0000	-1.0000	2.0000	
1	1.5000	0.8750	5.7500	0.1522
2	1.3478	0.1007	4.4499	0.0226
3	1.3252	0.0021	4.2685	0.0005
4	1.3247	0.0000	4.2646	0.0000
5	1.3247	0.0000	4.2646	0.0000

Example

Use Newton's Method to find a root of :

$$f(x) = e^{-x} - x$$

Use the initial point : $x_0 = 1.$

Stop after three iterations, or

if $\left| x_{k+1} - x_k \right| < 0.001,$ or

if $\left| f(x_k) \right| < 0.0001.$

Example

Use Newton's Method to find a root of :

$$f(x) = e^{-x} - x, \qquad f'(x) = -e^{-x} - 1$$

x_k	$f(x_k)$	$f'(x_k)$	$\dfrac{f(x_k)}{f'(x_k)}$
1.0000	-0.6321	-1.3679	0.4621
0.5379	0.0461	-1.5840	-0.0291
0.5670	0.0002	-1.5672	-0.0002
0.5671	0.0000	-1.5671	-0.0000

Example

Estimates of the root of: x-cos(x)=0.

0.60000000000000	Initial guess
0.74401731944598	1 correct digit
0.73909047688624	4 correct digits
0.73908513322147	10 correct digits
0.73908513321516	14 correct digits

Example

In estimating the root of: ***x-cos(x)=0***, to get more than 13 correct digits:

- 4 iterations of Newton ($x_0=0.8$)
- 43 iterations of Bisection method (initial interval [0.6, 0.8])
- 5 iterations of Secant method ($x_0=0.6$, $x_1=0.8$)

Euler's Method

$$\frac{dy}{dx} = f(x,y), y(0) = y_0$$

$$\text{Slope} = \frac{Rise}{Run}$$

$$= \frac{y_1 - y_0}{x_1 - x_0}$$

$$= f(x_0, y_0)$$

$$y_1 = y_0 + f(x_0, y_0)(x_1 - x_0)$$

$$= y_0 + f(x_0, y_0)h$$

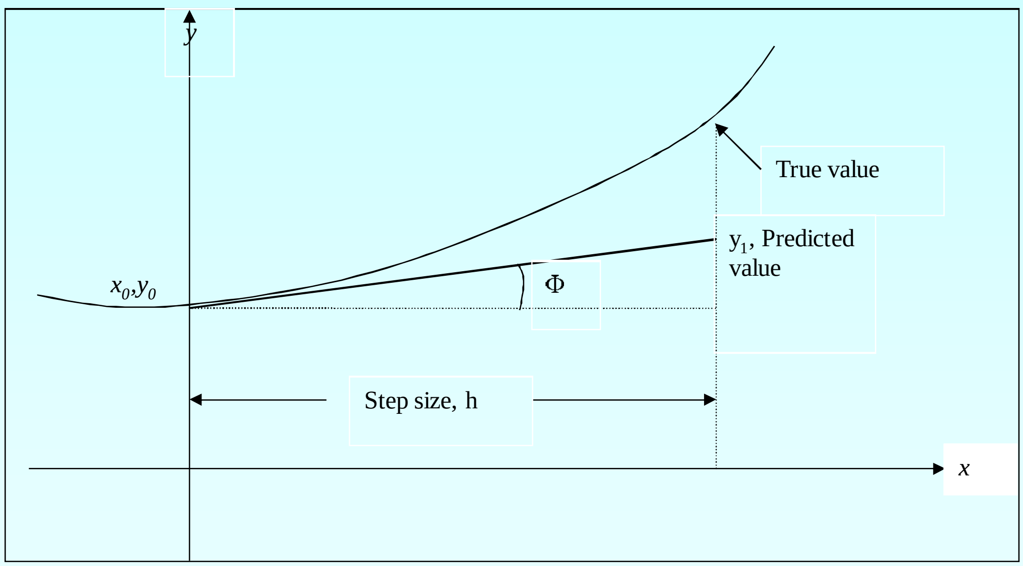


Figure 1 Graphical interpretation of the first step of Euler's method

Euler's Method

$$y_{i+1} = y_i + f\left(x_i, y_i\right)h$$

$$h = x_{i+1} - x_i$$

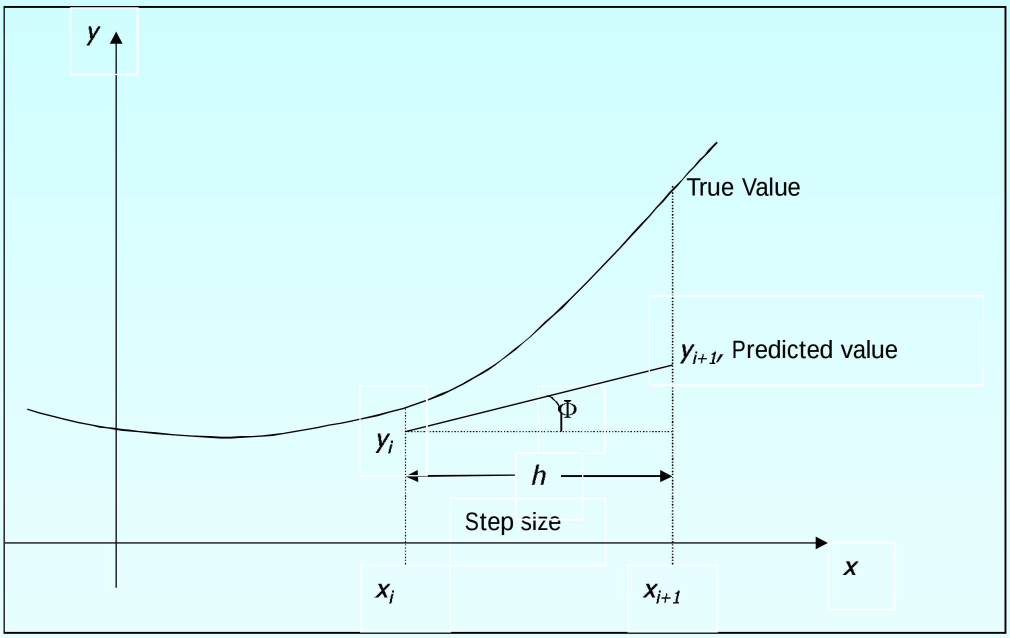


Figure 2. General graphical interpretation of Euler's method

How to write Ordinary Differential Equation

How does one write a first order differential equation in the form of

$$\frac{dy}{dx} = f(x, y)$$

Example

$$\frac{dy}{dx} + 2y = 1.3e^{-x}, \; y(0) = 5$$

is rewritten as

$$\frac{dy}{dx} = 1.3e^{-x} - 2y, \; y(0) = 5$$

In this case

$$f(x, y) = 1.3e^{-x} - 2y$$

Example

A ball at 1200K is allowed to cool down in air at an ambient temperature of 300K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right), \theta(0) = 1200\,K$$

Find the temperature at $t = 480$ seconds using Euler's method. Assume a step size of $h = 240$ seconds.

Solution

Step 1:

$$\frac{d\Theta}{dt} = -2.2067\times10^{-12}\left(\Theta^4 - 81\times10^8\right)$$

$$f\left(t,\Theta\right) = -2.2067\times10^{-12}\left(\Theta^4 - 81\times10^8\right)$$

$$\theta_{i+1} = \theta_i + f\left(t_i,\theta_i\right)h$$

$$\begin{aligned}\theta_1 &= \theta_0 + f\left(t_0,\theta_0\right)h\\ &= 1200 + f\left(0,1200\right)240\\ &= 1200 + \left(-2.2067\times10^{-12}\left(1200^4 - 81\times10^8\right)\right)240\\ &= 1200 + \left(-4.5579\right)240\\ &= 106.09K\end{aligned}$$

θ_1 is the approximate temperature at $t = t_1 = t_0 + h = 0 + 240 = 240$

$$\theta\left(240\right) \approx \theta_1 = 106.09K$$

Solution Cont

Step 2: For $i=1, \quad t_1 = 240, \quad \theta_1 = 106.09$

$$\begin{aligned}
\theta_2 &= \theta_1 + f(t_1, \theta_1)h \\
&= 106.09 + f(240, 106.09)240 \\
&= 106.09 + \left(-2.2067 \times 10^{-12}\left(106.09^4 - 81 \times 10^8\right)\right)240 \\
&= 106.09 + (0.017595)240 \\
&= 110.32K
\end{aligned}$$

θ_2 is the approximate temperature at $t = t_2 = t_1 + h = 240 + 240 = 480$

$$\theta(480) \approx \theta_2 = 110.32K$$

Solution Cont

The exact solution of the ordinary differential equation is given by the solution of a non-linear equation as

$$0.92593\ln\frac{\theta-300}{\theta+300}-1.8519\tan^{-1}(0.00333\theta)=-0.22067\times10^{-3}t-2.9282$$

The solution to this nonlinear equation at t=480 seconds is

$$\theta(480)=647.57K$$

Comparison of Exact and Numerical Solutions

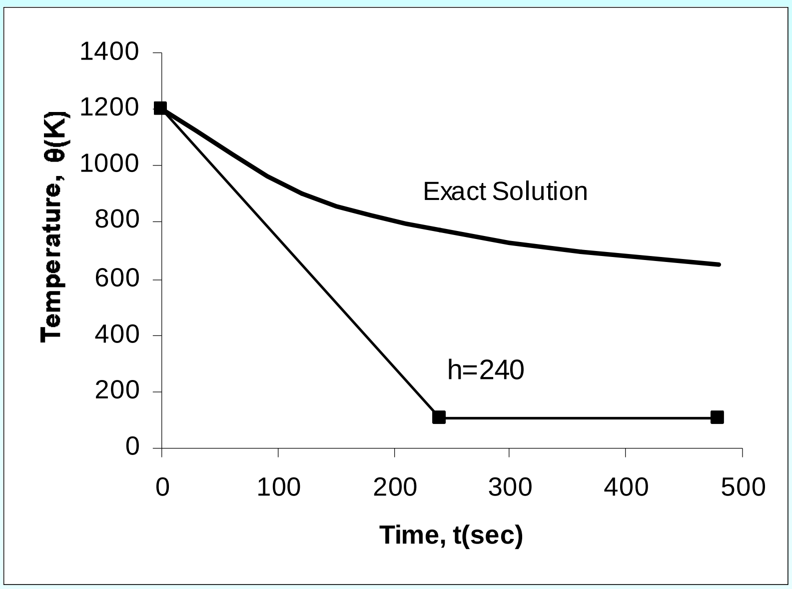


Figure 3. Comparing exact and Euler's method

Effect of step size

Table 1. Temperature at 480 seconds as a function of step size, h

Step, h	$\theta(480)$	E_t	$\lvert\epsilon_t\rvert\%$
480	−987.81	1635.4	252.54
240	110.32	537.26	82.964
120	546.77	100.80	15.566
60	614.97	32.607	5.0352
30	632.77	14.806	2.2864

$\theta(480) = 647.57K$ (exact)

Comparison with exact results

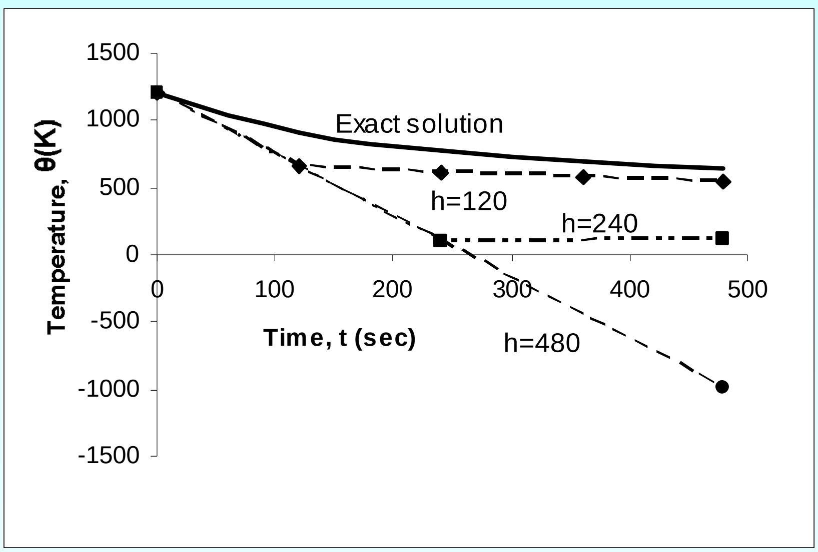


Figure 4. Comparison of Euler's method with exact solution for different step sizes

Effects of step size on Euler's Method

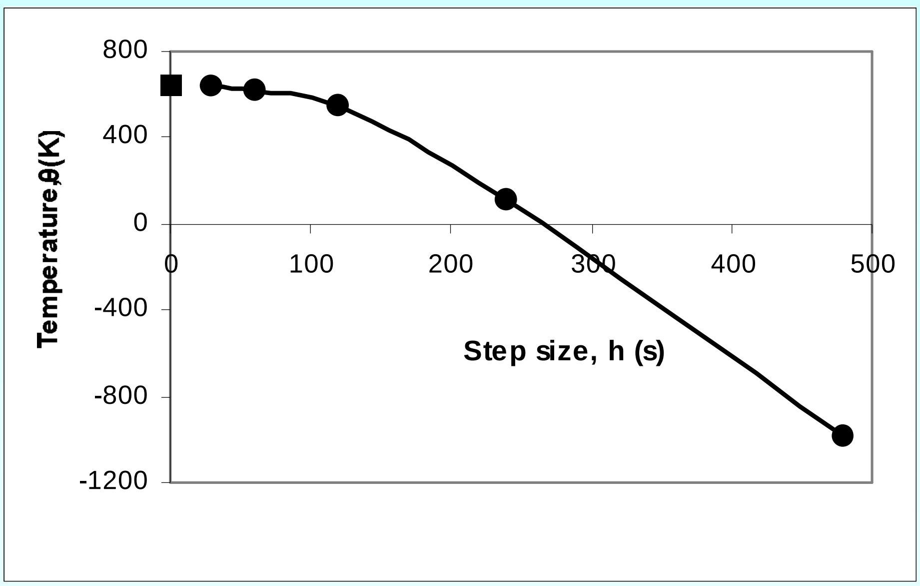


Figure 5. Effect of step size in Euler's method.

Errors in Euler's Method

It can be seen that Euler's method has large errors. This can be illustrated using Taylor series.

$$y_{i+1} = y_i + \left.\frac{dy}{dx}\right|_{x_i, y_i} (x_{i+1} - x_i) + \frac{1}{2!}\left.\frac{d^2 y}{dx^2}\right|_{x_i, y_i} (x_{i+1} - x_i)^2 + \frac{1}{3!}\left.\frac{d^3 y}{dx^3}\right|_{x_i, y_i} (x_{i+1} - x_i)^3 + \ldots$$

$$y_{i+1} = y_i + f(x_i, y_i)(x_{i+1} - x_i) + \frac{1}{2!} f'(x_i, y_i)(x_{i+1} - x_i)^2 + \frac{1}{3!} f''(x_i, y_i)(x_{i+1} - x_i)^3 + \ldots$$

As you can see the first two terms of the Taylor series

$y_{i+1} = y_i + f(x_i, y_i)h$ are the Euler's method.

The true error in the approximation is given by

$$E_t = \frac{f'(x_i, y_i)}{2!} h^2 + \frac{f''(x_i, y_i)}{3!} h^3 + \ldots \qquad E_t \propto h^2$$

Numerical Solution of Ordinary Differential Equations

Ordinary Differential Equation (ODE)

1. The general form of an m^{th} order ordinary differential equation is given by

$$\varphi(x, y, y', y'', \cdots, y^{(m)}) = 0.$$

Ordinary Differential Equation (ODE)

1. The general form of an m^{th} order ordinary differential equation is given by

$$\varphi(x, y, y', y'', \cdots, y^{(m)}) = 0.$$

2. A linear differential equation of order m can be written as

$$a_0(x)y^{(m)}(x) + a_1(x)y^{(m-1)}(x) + \cdots + a_{m-1}(x)y'(x) + a_m(x)y(x) = r(x)$$

where $a_0(x), a_1(x), \cdots, a_m(x)$ and $r(x)$ are constants or continuous functions of x.

General Solution

The general solution of an m^{th} order ordinary differential equation can be written in an implicit form as

$$\psi(x, y, c_1, c_2, \cdots, c_m) = 0,$$

or, in an explicit form as

$$y = h\phi(x, c_1, c_2, \cdots, c_m)$$

where $c_1, c_2, \cdots, c_m$ are m arbitrary constants.

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where $c_1, c_2, \cdots, c_m$ are m arbitrary constants.

The m arbitrary constants $c_1, c_2, \cdots, c_m$ can be determined by prescribing m conditions of the form
$y(x_0) = b_0, y'(x_0) = b_1, y''(x_0) = b_2, \cdots, y^{(m-1)}(x_0) = b_{m-1}$.

Initial Value Problem (IVP)

The m^{th} order ordinary differential equation

$$\varphi(x, y, y', y'', \cdots, y^{(m)}) = 0$$

together with the initial conditions

$$y(x_0) = b_0, y'(x_0) = b_1, y''(x_0) = b_2, \cdots, y^{(m-1)}(x_0) = b_{m-1}$$

is called an initial value problem.

Example

- Let us consider the second order initial value problem be given as

$$a_0(x)y''(x) + a_1(x)y'(x) + a_2(x)y(x) = r(x), \quad y(x_0) = b_0, y'(x_0) = b_1.$$

Example

- Let us consider the second order initial value problem be given as

$$a_0(x)y''(x) + a_1(x)y'(x) + a_2(x)y(x) = r(x), \quad y(x_0) = b_0, y'(x_0) = b_1.$$

- Define $u_1 = y$. Then we have

$$u_1(x_0) = b_0, \;\; u_1' = y' = u_2 (= f_1(x, u_1, u_2)) \;\; (say)$$

$$u_2' = y'' = \frac{1}{a_0(x)} [r(x) - a_1(x)u_2 - a_2(x)u_1] = f_2(x, u_1, u_2).\ (say)$$

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$$u_1(x_0) = b_0, \ u_1' = y' = u_2 (= f_1(x, u_1, u_2)) \ \ (say)$$
$$u_2' = y'' = \frac{1}{a_0(x)}[r(x) - a_1(x)u_2 - a_2(x)u_1] = f_2(x, u_1, u_2). \ (say)$$

- The system can be written as

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}' = \begin{pmatrix} f_1(x, u_1, u_2) \\ f_2(x, u_1, u_2) \end{pmatrix}, \ \begin{pmatrix} u_1(x_0) \\ u_2(x_0) \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}.$$

Reduction of m^{th} order initial value problem

- In general, we may have a system as

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}' = \begin{pmatrix} f_1(x, y_1, y_2) \\ f_2(x, y_1, y_2) \end{pmatrix}, \begin{pmatrix} y_1(x_0) \\ y_2(x_0) \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}$$

$$\overline{y}' = \overline{f}(x, \overline{y}), \ \overline{y}(x_0) = \overline{b}.$$

Reduction of m^{th} order initial value problem

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$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}' = \begin{pmatrix} f_1(x, y_1, y_2) \\ f_2(x, y_1, y_2) \end{pmatrix}, \begin{pmatrix} y_1(x_0) \\ y_2(x_0) \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}$$

$$\overline{y}' = \overline{f}(x, \overline{y}), \ \overline{y}(x_0) = \overline{b}.$$

- Therefore, the methods derived for the solution of the first order initial value problem

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0$$

can be used to solve the the second order initial value problem by writing the method in vector form, and hence the m^{th} order initial value problem.

Definition (Numerical methods)

1. Divide the interval $[x_0, b]$ on which the solution is desired, into a finite number of subintervals by the points

$$x_0 < x_1 < x_2 < \cdots < x_n = b.$$

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2. The points are called **mesh points or grid points**. The spacing between the points is given by

$$h_i = x_i - x_{i-1}, \quad i = 1, 2, \cdots, n.$$

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2. The points are called **mesh points or grid points**. The spacing between the points is given by

$$h_i = x_i - x_{i-1}, \quad i = 1, 2, \cdots, n.$$

3. For our discussions, we shall consider the case of uniform mesh only, i.e., $h_i = h_j$ for each $i, j = 1, 2, \cdots, n$.

Classified Solution Methods

- Consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0.$$

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  (i) Single Step Methods (ii) Multi Step Methods

Classified Solution Methods

- Consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0.$$

- To find numerical solution of above problem, there are two types of methods:

  (i) Single Step Methods (ii) Multi Step Methods

- Denote the numerical solution and the exact solution at x_i by y_i and $y(x_i)$, respectively.

Single Step Methods

Important Points

- The solution at any point x_{i+1} is obtained using the solution at only the previous point x_i.

Single Step Methods

Important Points

- The solution at any point x_{i+1} is obtained using the solution at only the previous point x_i.
- A general single step method can be written as

$$y_{i+1} = y_i + h\varphi(x_{i+1}, x_i, y_{i+1}, y_i, h)$$

where φ is a function of the arguments $x_{i+1}, x_i, y_{i+1}, y_i, h$ and depends on the right hand side $f(x, y)$ of the given differential equation. This function φ is called the increment function.

Important Points

- **Local Truncation Error**: The Truncation error (T.E.) is defined by

$$T_{i+1} = y(x_{i+1}) - y(x_i) - h\varphi(x_{i+1}, x_i, y(x_{i+1}), y(x_i), h),$$

where the exact solution $y(x_i)$ satisfies the following equation:

$$y(x_{i+1}) = y(x_i) + h\varphi(x_{i+1}, x_i, y(x_{i+1}), y(x_i), h) + T_{i+1}.$$

Important Points

- **Local Truncation Error**: The Truncation error (T.E.) is defined by

$$T_{i+1} = y(x_{i+1}) - y(x_i) - h\varphi(x_{i+1}, x_i, y(x_{i+1}), y(x_i), h),$$

where the exact solution $y(x_i)$ satisfies the following equation:

$$y(x_{i+1}) = y(x_i) + h\varphi(x_{i+1}, x_i, y(x_{i+1}), y(x_i), h) + T_{i+1}.$$

- **Order of a Method**: The order of a method is the largest integer p for which

$$\frac{1}{h} T_{i+1} = O(h^p).$$

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$$y(x) = y(x_i) + (x - x_i)y'(x_i) + \frac{1}{2!}(x - x_i)^2 y''(x_i) + \cdots + \frac{1}{p!}(x - x_i)^p y^{(p)}(x_i) + \frac{1}{(p+1)!}(x - x_i)^{p+1} y^{(p+1)}(x_i + \theta h)$$

where $0 < \theta < 1, x \in [x_0, b]$ and b is the point up to which the solution is required.

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Neglecting the error term, we obtain the Taylor series method as

$$y_{i+1} = y_i + hy_i' + \frac{1}{2!}h^2 y_i'' + \cdots + \frac{1}{p!}h^p y_i^{(p)}$$

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The bound on the truncation error of the Taylor series method of order p is given by

$$|T_{i+1}| = \left| \frac{1}{(p+1)!} h^{p+1} y^{(p+1)}(x_i + \theta h) \right| \leq \frac{1}{(p+1)!} h^{p+1} M_{p+1}.$$

where

$$M_{p+1} = max_{x \in [x_0, b]} |y^{(p+1)}(x)|.$$

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Compute an approximation to $y(1)$, $y'(1)$ and $y''(1)$ with Taylor's algorithm of order two and step length $h = 1$ when $y(x)$ is the solution to the initial value problem

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Consider the initial value problem $y' = x(y+x) - 2, y(0) = 2$. Use Euler's Method with step sizes $h = 0.3, h = 0.2$ and $h = 0.15$ to compute approximations to $y(0.6)$(5 decimals).

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$h = 0.15$:

$n = 0, x_0 = 0 : \; y_1 = y_0 + 0.15[-2] = 2 - 0.3 = 1.7$

$n = 1, x_1 = 0.15 : \; y_2 = y_1 + 0.15[0.15(y_1 + 0.15) - 2] = 1.441625$

$n = 2, x_2 = 0.30 : \; y_3 = y_2 + 0.15[0.3(y_2 + 0.3) - 2] = 1.219998$

$n = 3, x_3 = 0.45 : \; y_4 = y_3 + 0.15[0.45(y_3 + 0.45) - 2] = 1.032723$

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The integrand on the right hand side is the slope of the solution curve which changes continuously in $[x_i, x_{i+1}]$.

If we approximate the continuously varying slope in $[x_i, x_{i+1}]$ by a fixed slope or by a linear combination of slopes at several points in $[x_i, x_{i+1}]$, we obtain different methods.

CASE I:

Let $\theta = 0$. In this case, we are approximating the continuously varying slope in $[x_i, x_{i+1}]$ by the fixed slope at x_i. We obtain the method

$$y_{i+1} = y_i + hf(x_i, y_i),$$

which is the Euler method. The method is of first order.

CASE II:

Let $\theta = 1$. In this case, we are approximating the continuously varying slope in $[x_i, x_{i+1}]$ by the fixed slope at x_{i+1}. We obtain the method

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$$y_{i+1} = y_i + hf(x_{i+1}, y_i + hf(x_i, y_i)).$$

CASE III:

Let $\theta = 1/2$. In this case, we are approximating the continuously varying slope in $[x_i, x_{i+1}]$ by the fixed slope at $x_{i+1/2}$. We obtain the method

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$$\begin{aligned}
T.E. =& y_{i+1} - y_i - hf\left(x_{i+1}, y_i + \frac{h}{2} f(x_i, y_i)\right) \\
=& \left[y + hy' + \frac{h^2 y''}{2} + \frac{h^3 y''}{3!} + \cdots\right](x_i, y_i) - y_i \\
& - h\left[f + \frac{h}{2} f_x + \frac{h}{2} ff_x + (\text{three} \quad \text{terms} \quad \text{of} h^2) + \cdots\right](x_i, y_i) \\
=& \left[y + hf + \frac{h^2}{2}(f_x + ff_y) + (\text{five} \quad \text{terms} \quad \text{of} h^2) + \cdots\right](x_i, y_i) - y_i \\
& - h\left[f + \frac{h}{2} f_x + \frac{h}{2} ff_x + (\text{three} \quad \text{terms} \quad \text{of} h^2) + \cdots\right](x_i, y_i) \\
=& (\text{three} \quad \text{terms} \quad \text{of } h^3) + \cdots
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The truncation error in the method is given by

$$\begin{aligned}
T.E. =& y_{i+1} - y_i - hf\left(x_{i+1}, y_i + \frac{h}{2} f(x_i, y_i)\right)\\
=& \left[y + hy' + \frac{h^2 y''}{2} + \frac{h^3 y''}{3!} + \cdots\right](x_i, y_i) - y_i\\
& - h\left[f + \frac{h}{2} f_x + \frac{h}{2} ff_x + (\text{three} \quad \text{terms} \quad \text{of} h^2) + \cdots\right](x_i, y_i)\\
=& \left[y + hf + \frac{h^2}{2}(f_x + ff_y) + (\text{five} \quad \text{terms} \quad \text{of} h^2) + \cdots\right](x_i, y_i) - y_i\\
& - h\left[f + \frac{h}{2} f_x + \frac{h}{2} ff_x + (\text{three} \quad \text{terms} \quad \text{of} h^2) + \cdots\right](x_i, y_i)\\
=& (\text{three} \quad \text{terms} \quad \text{of } h^3) + \cdots
\end{aligned}$$

The truncation error is of order $O(h^3)$. Therefore, the method is of second order.

CASE IV:

Let the continuously varying slope in $[x_i, x_{i+1}]$ be approximated by the mean of slopes at the points x_i and x_{i+1}. Then, we obtain the method

$$y_{i+1} = y_i + \frac{h}{2}\left[f(x_i, y_i) + f(x_{i+1}, y_{i+1})\right].$$

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=& \left[y + hy' + \frac{h^2 y''}{2} + \frac{h^3 y''}{3!} + \cdots\right](x_i, y_i) - y_i \\
& - \frac{h}{2}\left[2f + hf_x + hff_x + (\text{three} \quad \text{terms} \quad \text{of } h^2) + \cdots\right](x_i, y_i) \\
=& \left[y + hf + \frac{h^2}{2}(f_x + ff_y) + (\text{five} \quad \text{terms} \quad \text{of } h^2) + \cdots\right](x_i, y_i) - y_i \\
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=& (\text{three} \quad \text{terms} \quad \text{of } h^3) + \cdots
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The truncation error is of order $O(h^3)$. Therefore, the method is of second order.

Problem: Apply the Euler-Cauchy method with step length h to the problem $y\prime = -y, y(0) = 1$. Determine an explicit expression for y_n.

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$$\begin{aligned} K_1 =& hf(x_n, y_n), K_2 = hf(x_n + h, y_n + K_1) \\ y_{n+1} =& y_n + \frac{1}{2}(K_1 + K_2). \end{aligned}$$

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If we apply to the differential equation $y\prime = -y$ we get

$$K_1 = -hy_n, K_2 = -h(y_n - hy) = -h(1 - h)y_n$$

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The solution of the differential equation satisfying the initial condition $y(0) = 1$ is given by

$$y_n = \left(1 - h + \frac{1}{2}h^2\right)^n, n = 0, 1, \ldots$$

Runge-Kutta Method of Second Order

Define

$$\begin{aligned} k_1 &= hf(x_i, y_i) \\ k_2 &= hf(x_i + c_2 h, y_i + a_{21} k_1) \\ y_{i+1} &= y_i + w_1 k_1 + w_2 k_2 \end{aligned}$$

where the values of the parameters c_2, a_{21}, w_1, w_2 are chosen such that the method is of highest possible order.

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where the values of the parameters c_2, a_{21}, w_1, w_2 are chosen such that the method is of highest possible order.
Observe that

$$\begin{aligned} k_2 =& hf(x_i + c_2 h, y_i + a_{21} k_1) \\ =& [f + h(c_2 f_x + a_{21} ff_y) + \frac{h^2}{2}(f_x + ff_y) \\ &+ \frac{h^3}{2!}(c_2^2 f_{xx} + a_{21}^2 f^2 f_{yy} + 2c_2 a_{21} ff_{xy}) + \cdots](x_i, y_i). \end{aligned}$$

Hence

$$
\begin{aligned}
y_{i+1} =& y_i + w_1 k_1 + w_2 k_2 \\
=& y_i + w_1 f(x_i, y_i) + hf(x_i + c_2 h, y_i + a_{21} k_1) \\
=& y_i + (w_1 + w_2) hf + h^2 (w_2 c_2 f_x + w_2 a_{21} ff_y) \\
&+ \frac{h^3}{2!} w_2 (c_2^2 f_{xx} + a_{21}^2 f^2 f_{yy} + 2c_2 a_{21} ff_{xy}) + \cdots](x_i, y_i),
\end{aligned}
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Hence

$$\begin{aligned}
y_{i+1} =& y_i + w_1 k_1 + w_2 k_2 \\
=& y_i + w_1 f(x_i, y_i) + hf(x_i + c_2 h, y_i + a_{21} k_1) \\
=& y_i + (w_1 + w_2)hf + h^2(w_2 c_2 f_x + w_2 a_{21} ff_y) \\
&+ \frac{h^3}{2!} w_2(c_2^2 f_{xx} + a_{21}^2 f^2 f_{yy} + 2c_2 a_{21} ff_{xy}) + \cdots](x_i, y_i),
\end{aligned}$$

Taylor series expansion about x = xi, gives

$$\begin{aligned}
y(x_{i+1}) =& y(x_i) + hy'(x_i) + \frac{h^2}{2} y''(x_i) + \frac{h^3}{3!} y'''(x_i) + \cdots \\
=& y(x_i) + hf(x_i, y_i) + \frac{h^2}{2}(f_x + ff_y)(x_i, y_i) \\
&+ \frac{h^3}{3!}\left[f_{xx} + f^2 f_{yy} + 2ff_{xy} + f_y(f_x + ff_y)\right](x_i, y_i) + \cdots
\end{aligned}$$

Comparing the coefficients of h and h^2 in above both equations, we obtain

$$w_1 + w_2 = 1, c_2 w_2 = 1/2, a_{21} w_2 = 1/2.$$

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where c_2 is arbitrary.

Runge-Kutta methods using two slopes

The Runge-Kutta methods using two slopes is given by

$$y_{i+1} = y_i + \left(1 - \frac{1}{2c_2}\right) k_1 + \frac{1}{2c_2} k_2$$

$$\text{where} \quad k_1 = hf(x_i, y_i)$$

$$k_2 = hf(x_i + c_2 h, y_i + c_2 k_1), \text{ where } c_2 \text{ is an arbitrary parameter.}$$

For $c_2 = 1$, we get **Heun's method or Euler-Cauchy method**.

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Error of the Runge-Kutta method The truncation error in the method is

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Error of the Runge-Kutta method The truncation error in the method is

$$T.E. = y(x_{i+1}) - y_{i+1} \approx O(h^3)$$

The method is of second order for all values of c_2.

Runge-Kutta methods using four slopes

The Runge-Kutta methods using four slopes is given by

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$\begin{aligned} \textit{where} \quad k_1 &= hf(x_i, y_i) \\ k_2 &= hf(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}) \\ k_3 &= hf(x_i + \frac{h}{2}, y_i + \frac{k_2}{2}) \\ k_4 &= hf(x_i + h, y_i + k_3) \end{aligned}$$

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k_3 &= hf(x_i + \frac{h}{2}, y_i + \frac{k_2}{2}) \\
k_4 &= hf(x_i + h, y_i + k_3)
\end{aligned}
$$

The truncation error is of order $O(h^5)$. The method is called the classical Runge-Kutta method of fourth order.

Problem: Use the classical Runge-Kutta method of fourth order to find the numerical solution at $x = 0.8$ for

$$\frac{dy}{dx} = \sqrt{x + y}, y(0.4) = 0.41.$$

Assume the step length $h = 0.2$.

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Solution: For $n = 0$ and $h = 0.2$, we have

$$x_0 = 0.4, y_0 = 0.41$$

$$K_1 = hf(x_0, y_0) = 0.2(0.4 + 0.41)^{1/2} = 0.18,$$

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$$K_1 = hf(x_0, y_0) = 0.2(0.4 + 0.41)^{1/2} = 0.18,$$

$$K_2 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{K_1}{2}\right) = 0.2\left[0.4 + 0.1 + 0.41 + \frac{1}{2}(0.18)\right]^{1/2} = 0.2,$$

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$$K_3 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{K_2}{2}\right) = 0.2\left[0.4 + 0.1 + 0.41 + \frac{1}{2}(0.02)\right]^{1/2} = 0.2009975,$$

Problem: Use the classical Runge-Kutta method of fourth order to find the numerical solution at $x = 0.8$ for

$$\frac{dy}{dx} = \sqrt{x+y}, y(0.4) = 0.41.$$

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Solution: For $n = 0$ and $h = 0.2$, we have

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$$K_4 = hf\left(x_0 + h, y_0 + K_3\right) = 0.2\left[0.4 + 0.2 + 0.41 + 0.2009975\right]^{1/2} = 0.2200907,$$

Problem: Use the classical Runge-Kutta method of fourth order to find the numerical solution at $x = 0.8$ for

$$\frac{dy}{dx} = \sqrt{x + y}, y(0.4) = 0.41.$$

Assume the step length $h = 0.2$.

Solution: For $n = 0$ and $h = 0.2$, we have

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$$K_4 = hf(x_0 + h, y_0 + K_3) = 0.2[0.4 + 0.2 + 0.41 + 0.2009975]^{1/2} = 0.2200907,$$

$$y_1 = y_0 + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) = 0.6103476.$$

For $n = 1, x_1 = 0.6$ and $y_1 = 0.6103476$, we obtain

$$K_1 = 0.2200316, K_2 = 0.2383580, K_3 = 0.2391256, K_4 = 0.2568636,$$

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$$K_1 = 0.2200316, K_2 = 0.2383580, K_3 = 0.2391256, K_4 = 0.2568636,$$

$$y_2 = 0.6103476 + 0.2386436 = 0.8489913.$$

For $n = 1, x_1 = 0.6$ and $y_1 = 0.6103476$, we obtain

$$K_1 = 0.2200316, K_2 = 0.2383580, K_3 = 0.2391256, K_4 = 0.2568636,$$
$$y_2 = 0.6103476 + 0.2386436 = 0.8489913.$$

Hence, we have $y(0.6) = 0.61035, y(0.8) = 0.84899.$

Problem

Solve the system

$$\begin{aligned} \overline{y}' &= \overline{f}(x, \overline{y}) \\ \overline{y}(x_0) &= \overline{b}. \end{aligned}$$

OR

Problem

Solve the m^{th} order initial value problem:

$$a_0(x)y^{(m)}(x) + a_1(x)y^{(m-1)}(x) + \cdots + a_{m-1}(x)y'(x) + a_m(x)y(x) = r(x),$$

$$y(x_0) = b_0, y'(x_0) = b_1, y''(x_0) = b_2, \cdots, y^{(m-1)}(x_0) = b_{m-1},$$

where $a_0(x), a_1(x), \cdots, a_m(x)$ and $r(x)$ are constants or continuous functions of x.

Taylor Series Method for System of First Order IVP: The Taylor series method of order p is

$$\overline{y}_{i+1} = \overline{y}_i + h\overline{y}_i' + \frac{1}{2!}h^2\overline{y}_i'' + \cdots + \frac{1}{p!}h^p\overline{y}_i^{(p)}$$

where

Taylor Series Method for System of First Order IVP: The Taylor series method of order p is

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where

$$\overline{y}_i^{(k)} = \begin{pmatrix} \overline{y}_{1,i}^{(p)} \\ \overline{y}_{2,i}^{(p)} \end{pmatrix} = \begin{pmatrix} \frac{d^{k-1}}{dx^{k-1}} f_1(x, y_{1,i}, y_{2,i}) \\ \frac{d^{k-1}}{dx^{k-1}} f_2(x, y_{1,i}, y_{2,i}) \end{pmatrix}$$

Euler's method for solving the system is given by

$$\overline{y}_{i+1} = \overline{y}_i + h\overline{y}'_i = \overline{y}_i + h\overline{f}'(x_i, \overline{y}_i)$$

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In component form, we obtain

$$\begin{aligned}(y_1)_{i+1} =& (y_1)_i + h(y_1')_i = (y_1)_i + hf_1(x_i, (y_1)_i, (y_2)_i)\\ (y_2)_{i+1} =& (y_2)_i + h(y_2')_i = (y_2)_i + hf_2(x_i, (y_1)_i, (y_2)_i)\end{aligned}$$

Runge-Kutta methods of fourth Order

The Runge-Kutta methods using four slopes is given by

$$\overline{y}_{i+1} = \overline{y}_i + \frac{1}{6}(\overline{k}_1 + 2\overline{k}_2 + 2\overline{k}_3 + \overline{k}_4)$$

$$\textit{where} \quad \overline{k}_1 = h\overline{f}(x_i, \overline{y}_i)$$

$$\overline{k}_2 = h\overline{f}(x_i + \frac{h}{2}, \overline{y}_i + \frac{\overline{k}_1}{2})$$

$$\overline{k}_3 = h\overline{f}(x_i + \frac{h}{2}, \overline{y}_i + \frac{\overline{k}_2}{2})$$

$$\overline{k}_4 = h\overline{f}(x_i + h, \overline{y}_i + \overline{k}_3)$$

Problem

The solution of the system of equations

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

$$u' = -4y - 2u, u(0) = 1,$$

is to be obtained by the Runge-Kutta fourth order method.Can a step length $h = 0.1$ be used for integration.If so find the approximant values of $y(0.2)$ and $u(0.2)$.

Solution: We have

$$K_1 = hu_n$$

$$l_1 = h(4y_n - 2u_n)$$

$$K_2 = h\left[u_n + \frac{1}{2}(-4hy_n - 2hu_n)\right] = -2h^2 y_n + (h - h^2)u_n,$$

$$l_2 = (-4h + 4h^2)y_n - 2hu_n,$$

$$K_3 = (-2h^2 + 2h^3)y_n + (h - h^2)u_n,$$

$$l_3 = (-4h + 4h^2)y_n + (-2h + 2h^3)u_n,$$

$$K_4 = (-4h^2 + 4h^3)y_n + (h - 2h62 + 2h^4)u_n,$$

$$l_4 = (-4h + 8h^2 - 8h^4)y_n + (-2h + 4h^3 - 4h^4)u_n,$$

$$y_{n+1} = \left(1 - 2h^2 + \frac{4}{3}h^3\right) + \left(h - h^2 + \frac{1}{3}h^4\right) u_n$$

$$u_{n+1} = \left(-4h + 4h^2 - \frac{4}{3}h^4\right) + \left(1 - 2h - + \frac{4}{3}h^3 - \frac{2}{3}h^4\right) u_n,$$

or

$$\begin{bmatrix} y_{n+1} \\ u_{n+1} \end{bmatrix} = \begin{bmatrix} 1 - 2h^2 + (4/3)h^3 & h - h^2 + (1/3)h^4 \\ -4h + 4h^2 - (4/3)h^4 & 1 - 2h + (4/3)h^3 - (2/3)h^4 \end{bmatrix} \begin{bmatrix} y_n \\ u_n \end{bmatrix}$$

For $h = 0.1$,we obtain

$$\begin{bmatrix} y_{n+1} \\ u_{n+1} \end{bmatrix} = \begin{bmatrix} 0.98133 & 0.09003 \\ -0.36013 & 0.80127 \end{bmatrix} \begin{bmatrix} y_n \\ u_n \end{bmatrix} = \mathbf{A} \begin{bmatrix} y_n \\ u_n \end{bmatrix}$$

We find that the roots of the characteristic equation

$$\xi^2 - 1.7826\,\xi + 0.818733 = 0,$$

are complex with modulus $|\xi| \leq 0.9048$.Hence $h = 0.1$ is a suitable step length for the Runge-kutta method.
We have the following results.

$$n = 0, x_0 = 0 : \quad \begin{bmatrix} y_1 \\ u_1 \end{bmatrix} = \mathbf{A} \begin{bmatrix} y_0 \\ u_0 \end{bmatrix} = \mathbf{A} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1.07136 \\ 0.44114 \end{bmatrix}$$

$$n = 1, x_1 = 0.1 : \quad \begin{bmatrix} y_2 \\ u_2 \end{bmatrix} = \mathbf{A} \begin{bmatrix} y_1 \\ u_1 \end{bmatrix} = \mathbf{A} \begin{bmatrix} 1.07136 \\ 0.44114 \end{bmatrix} = \begin{bmatrix} 1.09107 \\ -0.03236 \end{bmatrix}$$

Let us construct a few multi step methods.

Integrating the differential equation $y' = f(x, y)$ in the interval $[x_i, x_{i+1}]$, we get

$$\int_{x_i}^{x_{i+1}} \frac{dy}{dx}\, dx = \int_{x_i}^{x_{i+1}} f(x, y)\, dx.$$

or
$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y)\, dx. \tag{4.69}$$

To derive the methods, we approximate the integrand $f(x, y)$ by a suitable interpolation polynomial.

In general, we may integrate the differential equation $y' = f(x, y)$ in the interval $[x_{i-m}, x_{i+1}]$. We get

$$\int_{x_{i-m}}^{x_{i+1}} \frac{dy}{dx}\, dx = \int_{x_{i-m}}^{x_{i+1}} f(x, y)\, dx$$

or
$$y(x_{i+1}) = y(x_{i-m}) + \int_{x_{i-m}}^{x_{i+1}} f(x, y)\, dx.$$

For $m = 0$, we get (4.69).

4.6.1 Predictor Methods (Adams-Bashforth Methods)

All predictor methods are explicit methods.

We have k data values, $(x_i, f_i)(x_{i-1}, f_{i-1})$, ..., (x_{i-k+1}, f_{i-k+1}). For this data, we fit the Newton's backward difference interpolating polynomial of degree $k - 1$ as (see equation (2.47) in chapter 2)

$$P_{k-1}(x) = f(x_i + sh) = f(x_i) + s\nabla f(x_i) + \frac{s(s+1)}{2!} \nabla^2 f(x_i) + \ldots$$

$$+ \frac{s(s+1)(s+2) \ldots (s+k-2)}{(k-1)!} \nabla^{k-1} f(x_i). \tag{4.70}$$

Note that $s = [(x - x_i)/h] < 0.$

The expression for the error is given by

$$\text{T.E.} = \frac{s(s+1)(s+2) \ldots (s+k-1)}{(k)!} h^k f^{(k)}(\xi) \tag{4.71}$$

where ξ lies in some interval containing the points $x_i, x_{i-1}, \ldots, x_{i-k+1}$ and x. We replace $f(x, y)$ by $P_{k-1}(x)$ in (4.69). The limits of integration in (4.69) become

for $x = x_i$, $s = 0$ and for $x = x_{i+1}$, $s = 1$.

Also, $dx = hds$. We get

$$y_{i+1} = y_i + h \int_0^1 \left[f_i + s\nabla f_i + \frac{1}{2} s(s+1)\nabla^2 f_i + \frac{1}{6} s(s+1)(s+2)\nabla^3 f_i + \ldots \right] ds$$

Now, $$\int_0^1 s\,dx = \frac{1}{2}, \quad \int_0^1 s(s+1)\,ds = \frac{5}{6},$$

$$\int_0^1 s(s+1)(s+2)\,ds = \frac{9}{4}, \quad \int_0^1 s(s+1)(s+2)(s+3)\,ds = \frac{251}{30}.$$

Hence, we have

$$y_{i+1} = y_i + h\left[f_i + \frac{1}{2}\nabla f_i + \frac{5}{12}\nabla^2 f_i + \frac{3}{8}\nabla^3 f_i + \frac{251}{720}\nabla^4 f_i + \ldots\right]. \tag{4.72}$$

These methods are called *Adams-Bashforth methods.*

Using (4.71), we obtain the error term as

$$T_k = h^{k+1}\int_0^1 \frac{s(s+1)(s+2)\ldots(s+k-1)}{(k)!}\, f^{(k)}(\xi)\,ds$$

$$= h^{k+1}\int_0^1 g(s)\, f^{(k)}(\xi)\,ds. \tag{4.73}$$

Since, $g(s)$ does not change sign in [0, 1], we get by the mean value theorem

$$T_k = h^{k+1} f^{(k)}(\xi_1)\int_0^1 g(s)ds, \quad 0 < \xi_1 < 1 \tag{4.74}$$

where $$g(s) = \frac{1}{k!}\,[s(s+1)\ldots(s+k-1)].$$

Alternately, we write the truncation error as

$$\text{T.E.} = y(x_{n+1}) - y_{n+1}$$

Using Taylor series, we expand $y(x_{n+1})$, y_{n+1} about x_n, and simplify. The leading term gives the order of the truncation error.

Remark 8 From (4.74), we obtain that the truncation error is of order $O(h^{k+1})$. Therefore, a k-step Adams-Bashforth method is of order k.

By choosing different values for k, we get different methods.

$k = 1$: We get the method

$$y_{i+1} = y_i + hf_i \tag{4.75}$$

which is the Euler's method. Using (4.74), we obtain the error term as

$$T_1 = \frac{h^2}{2} f'(\xi_1) = \frac{h^2}{2} y''(\xi_1).$$

Therefore, the method is of first order.

$k = 2$: We get the method

$$y_{i+1} = y_i + h\left[f_i + \frac{1}{2}\nabla f_i\right] = y_i + h\left[f_i + \frac{1}{2}(f_i - f_{i-1})\right]$$

$$= y_i + \frac{h}{2}\,[3f_i - f_{i-1}]. \tag{4.76}$$

For using the method, we require the starting values y_i and y_{i-1}.

Using (4.74), we obtain the error term as

$$T_2 = \frac{5}{12} h^3 f''(\xi_2) = \frac{5}{12} h^3 y'''(\xi_2).$$

Therefore, the method is of second order.

$k = 3$: We get the method

$$y_{i+1} = y_i + h\left[f_i + \frac{1}{2}\nabla f_i + \frac{5}{12}\nabla^2 f_i\right]$$

$$= y_i + h\left[f_i + \frac{1}{2}(f_i - f_{i-1}) + \frac{5}{12}(f_i - 2f_{i-1} + f_{i-2})\right]$$

$$= y_i + \frac{h}{12}\,[23f_i - 16f_{i-1} + 5f_{i-2}]. \tag{4.77}$$

For using the method, we require the starting values y_i, y_{i-1} and y_{i-2}.

Using (4.74), we obtain the error term as

$$T_3 = \frac{3}{8} h^4 f^{(3)}(\xi_3) = \frac{3}{8} h^4 y^{(4)}(\xi_3).$$

Therefore, the method is of third order.

$k = 4$: We get the method

$$y_{i+1} = y_i + h\left[f_i + \frac{1}{2}\nabla f_i + \frac{5}{12}\nabla^2 f_i + \frac{3}{8}\nabla^3 f_i\right]$$

$$= y_i + h\left[f_i + \frac{1}{2}(f_i - f_{i-1}) + \frac{5}{12}(f_i - 2f_{i-1} + f_{i-2}) + \frac{3}{8}(f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3})\right]$$

$$= y_i + \frac{h}{24}\,[55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}]. \tag{4.78}$$

For using the method, we require the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}.

Using (4.74), we obtain the error term as

$$T_4 = \frac{251}{720} h^5 f^{(4)}(\xi_4) = \frac{251}{720} h^5 y^{(5)}(\xi_4).$$

Therefore, the method is of fourth order.

Remark 9 The required starting values for the application of the Adams-Bashforth methods are obtained by using any single step method like Euler's method, Taylor series method or Runge-Kutta method.

Example 4.12 *Find the approximate value of* $y(0.3)$ *using the Adams-Bashforth method of third order for the initial value problem*

$$y' = x^2 + y^2,\ y(0) = 1$$

with $h = 0.1$. *Calculate the starting values using the corresponding Taylor series method with the same step length.*

Solution We have $f(x, y) = x^2 + y^2$, $x_0 = 0$, $y_0 = 1$.

The Adams-Bashforth method of third order is given by

$$y_{i+1} = y_i + \frac{h}{12}[23f_i - 16f_{i-1} + 5f_{i-2}].$$

We need the starting values, y_0, y_1, y_2. The initial condition gives $y_0 = 1$.

The third order Taylor series method is given by

$$y_{i+1} = y_i + hy_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{6} y_i'''.$$

We have $\quad y' = x^2 + y^2,\ y'' = 2x + 2yy',\ y''' = 2 + 2[yy'' + (y')^2].$

We obtain the following starting values.

$$i = 0 : x_0 = 0,\ y_0 = 1,\ y_0' = 1,\ y_0'' = 2,\ y_0''' = 8.$$

$$y(0.1) \approx y_1 = y_0 + 0.1\, y_0' + \frac{0.01}{2} y_0'' + \frac{0.001}{6} y_0'''$$

$$= 1 + 0.1(1) + 0.005(2) + \frac{0.001}{6}(8) = 1.111333.$$

$$i = 1: x_1 = 0.1,\ y_1 = 1.111333,\ y_1' = 1.245061,$$

$$y_1'' = 2.967355,\ y_1''' = 11.695793.$$

$$y(0.2) \approx y_2 = y_1 + 0.1\, y_1' + \frac{0.01}{2} y_1'' + \frac{0.001}{6} y_1'''$$

$$= 1.111333 + 0.1(1.245061) + 0.005\,(2.967355) + \frac{0.001}{6}(11.695793)$$

$$= 1.252625.$$

Now, we apply the given Adams-Bashforth method. We have

$$x_2 = 0.2,\ y_2 = 1.252625,\ y_2' = f_2 = 1.609069.$$

For $i = 2$, we obtain

$$y(0.3) \approx y_3 = y_2 + \frac{h}{12}[23f_2 - 16f_1 + 5\,f_0]$$

$$= y_2 + \frac{0.1}{12}[23(1.609069) - 16(1.245061) + 5(1)] = 1.436688.$$

Example 4.13 *Find the approximate value of* $y(0.4)$ *using the Adams-Bashforth method of fourth order for the initial value problem*

$$y' = x + y^2,\ y(0) = 1$$

with $h = 0.1$. *Calculate the starting values using the Euler's method with the same step length.*

Solution We have $f(x, y) = x + y^2$, $x_0 = 0$, $y_0 = 1$.

The Adams-Bashforth method of fourth order is given by

$$y_{i+1} = y_i + \frac{h}{24}\,[55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}].$$

We need the starting values, y_0, y_1, y_2, y_3. The initial condition gives $y_0 = 1$.

Euler's method is given by

$$y_{i+1} = y_i + h\,y_i' = y_i + h\,f_i.$$

We obtain the following starting values.

$i = 0$: $\quad x_0 = 0,\ y_0 = 1,\ y_0' = f_0 = 1.$

$$y(0.1) \approx y_1 = y_0 + 0.1\,y_0' = 1 + 0.1(1) = 1.1.$$

$i = 1$: $\quad x_1 = 0.1,\ y_1 = 1.1,\ y_1' = f(0.1, 1.1) = 1.31.$

$$y(0.2) \approx y_2 = y_1 + 0.1\,y_1' = 1.1 + 0.1(1.31) = 1.231.$$

$i = 2$: $\quad x_2 = 0.2,\ y_2 = 1.231,\ y_2' = f(0.2, 1.231) = 1.715361.$

$$y(0.3) \approx y_3 = y_2 + 0.1\,y_2' = 1.231 + 0.1(1.715361) = 1.402536.$$

Now, we apply the given Adams-Bashforth method. We have

$$x_3 = 0.3,\ y_3 = 1.402536,\ y_3' = f_3 = 2.267107.$$

For $i = 3$, we obtain

$$\begin{aligned} y(0.4) \approx y_4 &= y_3 + \frac{0.1}{24}\,[55\,f_3 - 59f_2 + 37f_1 - 9f_0] \\ &= 1.402536 + \frac{0.1}{24}\,[55(2.267107) - 59(1.715361) + 37(1.31) - 9(1)] \\ &= 1.664847. \end{aligned}$$

4.6.2 Corrector Methods

All corrector methods are implicit methods.

4.6.2.1 Adams-Moulton Methods

Consider the $k + 1$ data values, (x_{i+1}, f_{i+1}), (x_i, f_i), (x_{i-1}, f_{i-1}), ..., (x_{i-k+1}, f_{i-k+1}) which include the current data point. For this data, we fit the Newton's backward difference interpolating polynomial of degree k as (see equation (2.47) in chapter 2)

$$P_k(x) = f(x_i + sh) = f(x_{i+1}) + (s-1)\,\nabla f(x_{i+1}) + \frac{(s-1)s}{2!}\,\nabla^2 f(x_{i+i}) + \ldots$$

$$+ \frac{(s-1)s(s+1)(s+2)\ldots(s+k-2)}{(k)!}\nabla^k\, f(x_{i+1}) \qquad (4.79)$$

where $\qquad s = [(x - x_i)/h] < 0.$

The expression for the error is given by

$$\text{T.E.} = \frac{(s-1)s(s+1)(s+2)\ldots(s+k-1)}{(k+1)!}\; h^{k+1} f^{(k+1)}(\xi) \qquad (4.80)$$

where ξ lies in some interval containing the points $x_{i+1}, x_i, \ldots, x_{n-k+1}$ and x. We replace $f(x, y)$ by $P_k(x)$ in (4.69). The limits of integration in (4.69) become

for $x = x_i$, $s = 0$, and for $x = x_{i+1}$, $s = 1$.

Also, $dx = hds$. We get

$$y_{i+1} = y_i + h\int_0^1 \left[f_{i+1} + (s-1)\,\nabla f_{i+1} + \frac{1}{2}(s-1)s\nabla^2 f_{i+1} \right.$$

$$\left. + \frac{1}{6}(s-1)s(s+1)\nabla^3 f_{i+1} + \ldots \right] ds$$

Now, $\qquad \int_0^1 (s-1)\,ds = -\frac{1}{2}, \quad \int_0^1 (s-1)s\,ds = \left[\frac{s^3}{3} - \frac{s^2}{2}\right]_0^1 = -\frac{1}{6}$

$$\int_0^1 (s-1)s(s+1)\,ds = \left[\frac{s^4}{4} - \frac{s^2}{2}\right]_0^1 = -\frac{1}{4}.$$

$$\int_0^1 (s-1)s(s+1)(s+2)\,ds = -\frac{19}{30}.$$

Hence, we have

$$y_{i+1} = y_i + h\left[f_{i+1} - \frac{1}{2}\nabla f_{i+1} - \frac{1}{12}\nabla^2 f_{i+1} - \frac{1}{24}\nabla^3 f_{i+1} - \frac{19}{720}\nabla^4 f_{i+1} - \ldots \right] \qquad (4.81)$$

These methods are called *Adams-Moulton methods.*

Using (4.80), we obtain the error term as

$$T_k = h^{k+2}\int_0^1 \frac{(s-1)s(s+1)(s+2)\ldots(s+k-1)}{(k+1)!}\; f^{(k+1)}(\xi)\,ds$$

$$= h^{k+2}\int_0^1 g(s)\, f^{(k+1)}(\xi)\,ds \qquad (4.82)$$

where $$g(s) = \frac{1}{(k+1)!}\ [(s-1)s(s+1) \ldots (s+k-1)].$$

Since $g(s)$ does not change sign in [0, 1], we get by the mean value theorem

$$T_k = h^{k+2} f^{(k+1)}(\xi_1) \int_0^1 g(s)\, ds,\quad 0 < \xi_1 < 1. \tag{4.83}$$

Remark 10 From (4.83), we obtain that the truncation error is of order $O(h^{k+2})$. Therefore, a k-step Adams-Moulton method is of order $k + 1$.

By choosing different values for k, we get different methods.

$k = 0$: We get the method

$$y_{i+1} = y_i + hf_{i+1} \tag{4.84}$$

which is the backward Euler's method. Using (4.83), we obtain the error term as

$$T_1 = -\frac{h^2}{2} f'(\xi_1) = -\frac{h^2}{2} y''(\xi_1).$$

Therefore, the method is of first order.

$k = 1$: We get the method

$$y_{i+1} = y_i + h\left[f_{i+1} - \frac{1}{2}\nabla f_{i+1}\right] = y_i + h\left[f_{i+1} - \frac{1}{2}(f_{i+1} - f_i)\right]$$

$$= y_i + \frac{h}{2}[f_{i+1} + f_i]. \tag{4.85}$$

This is also a single step method and we do not require any starting values. This method is also called the *trapezium method.*

Using (4.83), we obtain the error term as

$$T_2 = -\frac{1}{12} h^3 f''(\xi_2) = -\frac{1}{12} h^3 y'''(\xi_2).$$

Therefore, the method is of second order.

$k = 2$: We get the method

$$y_{i+1} = y_i + h\left[f_{i+1} - \frac{1}{2}\nabla f_{i+1} - \frac{1}{12}\nabla^2 f_{i+1}\right]$$

$$= y + h\left[f_{i+1} - \frac{1}{2}(f_{i+1} - f_i) - \frac{1}{12}(f_{i+1} - 2f_i + f_{i-1})\right]$$

$$= y_i + \frac{h}{12}[5f_{i+1} + 8f_i - f_{i-1}]. \tag{4.86}$$

For using the method, we require the starting values y_i, y_{i-1}.

Using (4.83), we obtain the error term as

$$T_3 = -\frac{1}{24} h^4 f^{(3)}(\xi_3) = -\frac{1}{24} h^4 y^{(4)}(\xi_3).$$

Therefore, the method is of third order.

$k = 3$: We get the method

$$y_{i+1} = y_i + h\left[f_{i+1} - \frac{1}{2}\nabla f_{i+1} - \frac{1}{12}\nabla^2 f_{i+1} - \frac{1}{24}\nabla^3 f_{i+1}\right]$$

$$= y_i + h\left[f_{i+1} - \frac{1}{2}(f_{i+1} - f_i) - \frac{1}{12}(f_{i+1} - 2f_i + f_{i-1})\right.$$

$$\left. - \frac{1}{24}(f_{i+1} - 3f_i + 3f_{i-1} - f_{i-2})\right]$$

$$= y_i + \frac{h}{24}[9f_{i+1} + 19f_i - 5f_{i-1} + f_{i-2}]. \tag{4.87}$$

For using the method, we require the starting values y_i, y_{i-1}, y_{i-2}.

Using (4.83), we obtain the error term as

$$T_4 = -\frac{19}{720} h^5 f^{(4)}(\xi_4) = -\frac{19}{720} h^5 y^{(5)}(\xi_4).$$

Therefore, the method is of fourth order.

4.6.2.2 Milne-Simpson Methods

To derive the Milne's methods, we integrate the differential equation $y' = f(x, y)$ in the interval $[x_{i-1}, x_{i+1}]$. We get

$$\int_{x_{i-1}}^{x_{i+1}} \frac{dy}{dx}\,dx = \int_{x_{i-1}}^{x_{i+1}} f(x, y)\,dx.$$

or

$$y(x_{i+1}) = y(x_{i-1}) + \int_{x_{i-1}}^{x_{i+1}} f(x, y)\,dx. \tag{4.88}$$

To derive the methods, we use the same approximation, follow the same procedure and steps as in Adams-Moulton methods. The interval of integration for s is $[-1, 1]$. We obtain

$$y_{i+1} = y_{i-1} + h\int_0^1 \left[f_{i+1} + (s-1)\nabla f_{i+1} + \frac{1}{2}(s-1)s\nabla^2 f_{i+1}\right.$$

$$\left. + \frac{1}{6}(s-1)s(s+1)\nabla^3 f_{i+1} + \ldots\right] ds$$

Now, $\int_{-1}^{1} (s-1)\, ds = -2, \quad \int_{0}^{1} (s-1)s\, ds = \frac{2}{3},$

$$\int_{-1}^{1} (s-1)s(s+1)\, ds = 0, \int_{-1}^{1} (s-1)s(s+1)(s+2)\, ds = -\frac{24}{90}.$$

Hence, we have

$$y_{i+1} = y_{i-1} + h\left[2f_{i+1} - 2\nabla f_{i+1} + \frac{1}{3}\nabla^2 f_{i+1} + (0)\nabla^3 f_{i+1} - \frac{1}{90}\nabla^4 f_{i+1} - \ldots\right]. \quad (4.89)$$

These methods are called *Milne's methods*.

The case $k = 2$, is of interest for us. We obtain the method as

$$y_{i+1} = y_{i-1} + h\left[2f_{i+1} - 2\nabla f_{i+1} + \frac{1}{3}\nabla^2 f_{i+1}\right]$$

$$= y_{i-1} + h\left[2f_{i+1} - 2(f_{i+1} - f_i) + \frac{1}{3}(f_{i+1} - 2f_i + f_{i-1})\right]$$

$$= y_{i-1} + \frac{h}{3}[f_{i+1} + 4f_i + f_{i-1})]. \quad (4.90)$$

This method is also called the *Milne-Simpson's method*.

For using the method, we require the starting values y_i, y_{i-1}.

The error term is given by

$$\text{Error} = -\frac{1}{90}h^5 f^{(4)}(\xi) = -\frac{1}{90}h^5 y^{(5)}(\xi).$$

Therefore, the method is of fourth order.

Remark 11 The methods derived in this section are all implicit methods. Therefore, we need to solve a nonlinear algebraic equation for obtaining the solution at each point. Hence, these methods are not used as such but in combination with the explicit methods. This would give rise to the explicit-implicit methods or predictor-corrector methods, which we describe in the next section.

4.6.2.3 Predictor-Corrector Methods

In the previous sections, we have derived explicit single step methods (Euler's method, Taylor series methods and Runge-Kutta methods), explicit multi step methods (Adams-Bashforth methods) and implicit methods (Adams-Moulton methods, Milne-Simpson methods) for the solution of the initial value problem $y' = f(x, y)$, $y(x_0) = y_0$. If we perform analysis for numerical stability of these methods (we shall discuss briefly this concept in the next section), we find that all explicit methods require very small step lengths to be used for convergence. If the solution of the problem is required over a large interval, we may need to use the method thousands or even millions of steps, which is computationally very expensive. Most implicit methods have strong stability properties, that is, we can use sufficiently large step lengths for computations and we can obtain convergence. However, we need to solve a nonlinear algebraic equation for the solution at each nodal point. This procedure may also be computationally expensive as convergence is to be obtained for the solution of the nonlinear equation at each nodal point. Therefore, we combine the explicit methods (which have weak stability properties) and implicit methods (which have strong stability properties) to obtain new methods. Such methods are called *predictor-corrector methods* or *P-C methods.*

Now, we define the predictor-corrector methods. We denote *P* for predictor and *C* for corrector.

P: Predict an approximation to the solution y_{i+1} at the current point, using an explicit method. Denote this approximation as $y_{i+1}^{(p)}$.

C: Correct the approximation $y_{i+1}^{(p)}$, using a corrector, that is, an implicit method. Denote this corrected value as $y_{i+1}^{(c)}$. The corrector is used 1 or 2 or 3 times, depending on the orders of explicit and implicit methods used.

Remark 12 The order of the predictor should be less than or equal to the order of the corrector. If the orders of the predictor and corrector are same, then we may require only one or two corrector iterations at each nodal point. For example, if the predictor and corrector are both of fourth order, then the combination (*P-C* method) is also of fourth order and we may require one or two corrector iterations at each point. If the order of the predictor is less than the order of the corrector, then we require more iterations of the corrector. For example, if we use a first order predictor and a second order corrector, then one application of the combination gives a result of first order. If corrector is iterated once more, then the order of the combination increases by one, that is the result is now of second order. If we iterate a third time, then the truncation error of the combination reduces, that is, we may get a better result. Further iterations may not change the results.

We give below a few examples of the predictor-corrector methods.

Example 1

Predictor P: Euler method:

$$y_{n+1}^{(p)} = y_n + hf(x_n, y_n). \tag{4.91}$$

$$\text{Error term} = \frac{h^2}{2} f'(\xi_1) = \frac{h^2}{2} y''(\xi_1).$$

Corrector C: Backward Euler method (4.84):

$$y_{n+1}^{(c)} = y_n + hf(x_{n+1}, y_{n+1}^{(p)}). \tag{4.92}$$

$$\text{Error term} = -\frac{h^2}{2} f'(\xi_1) = -\frac{h^2}{2} y''(\xi_1).$$

Both the predictor and corrector methods are of first order. We compute

$$y_{n+1}^{(0)} = y_n + hf(x_n, y_n).$$

$$y_{n+1}^{(1)} = y_n + hf(x_{n+1}, y_{n+1}^{(0)}).$$

$$y_{n+1}^{(2)} = y_n + hf(x_{n+1}, y_{n+1}^{(1)}), \text{ etc.}$$

Example 2

Predictor P: Euler method:

$$y_{n+1}^{(p)} = y_n + hf(x_n, y_n). \tag{4.93}$$

Corrector C: Trapezium method (4.85):

$$y_{n+1}^{(c)} = y_n + \frac{h}{2}[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(p)})]. \tag{4.94}$$

$$\text{Error term} = -\frac{1}{12}h^3 f''(\xi_2) = -\frac{1}{12}h^3 y'''(\xi_2).$$

The predictor is of first order and the corrector is of second order. We compute

$$y_{n+1}^{(0)} = y_n + hf(x_n, y_n).$$

$$y_{n+1}^{(1)} = y_n + \frac{h}{2}[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(0)})].$$

$$y_{n+1}^{(2)} = y_n + \frac{h}{2}[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(1)})], \text{ etc.}$$

Example 3 *Adams-Bashforth-Moulton predictor-corrector method of fourth order.*

Both the predictor and corrector methods are of fourth order.

Predictor P: Adams-Bashforth method of fourth order.

$$y_{i+1}^{(p)} = y_i + \frac{h}{24}[55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}]. \tag{4.95}$$

$$\text{Error term} = \frac{251}{720}h^5 f^{(4)}(\xi_4) = \frac{251}{720}h^5 y^{(5)}(\xi_4).$$

The method requires the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}.

Corrector C: Adams-Moulton method of fourth order.

$$y_{i+1}^{(c)} = y_i + \frac{h}{24}[9f(x_{i+1}, y_{i+1}^{(p)}) + 19f_i - 5f_{i-1} + f_{i-2}]. \tag{4.96}$$

$$\text{Error term} = -\frac{19}{720}h^5 f^{(4)}(\xi_4) = -\frac{19}{720}h^5 y^{(5)}(\xi_4).$$

The method requires the starting values y_i, y_{i-1}, y_{i-2}.

The combination requires the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}. That is, we require the values y_0, y_1, y_2, y_3. Initial condition gives the value y_0.

In the syllabus, this method is also referred to as *Adams-Bashforth predictor-corrector method.*

Example 4 *Milne's predictor-corrector method.*

Both the predictor and corrector methods are of fourth order.

Predictor P: Adams-Bashforth method of fourth order.

$$y_{i+1}^{(p)} = y_{i-3} + \frac{4h}{3}[2f_i - f_{i-1} + 2f_{i-2}]. \tag{4.97}$$

$$\text{Error term} = \frac{14}{45} h^5 f^{(4)}(\xi) = \frac{14}{45} h^5 y^{(5)}(\xi).$$

The method requires the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}.

Corrector C: Milne-Simpson's method of fourth order.

$$y_{i+1}^{(c)} = y_{i-1} + \frac{h}{3}[f(x_{i+1}, y_{i+1}^{(p)}) + 4f_i + f_{i-1})]. \tag{4.98}$$

$$\text{Error term} = -\frac{1}{90} h^5 f^{(4)}(\xi) = -\frac{1}{90} h^5 y^{(5)}(\xi).$$

The method requires the starting values y_i, y_{i-1}.

The combination requires the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}. That is, we require the values y_0, y_1, y_2, y_3. Initial condition gives the value y_0.

Remark 13 Method (4.97) is obtained in the same way as we have derived the Adams-Bashforth methods. Integrating the given differential equation $y' = f(x, y)$ on the interval (x_{i-3}, x_{i+1}), we obtain

$$\int_{x_{i-3}}^{x_{i+1}} \frac{dy}{dx}\, dx = \int_{x_{i-3}}^{x_{i+1}} f(x, y)\, dx$$

or

$$y(x_{i+1}) = y(x_{i-3}) + \int_{x_{i-3}}^{x_{i+1}} f(x, y)\, dx.$$

Replace the integrand on the right hand side by the same backward difference polynomial (4.70) and derive the method in the same way as we have done in deriving the explicit Adams-Bashforth methods. We obtain the method as

$$y_{i+1} = y_{i-3} + h\left[4f_i - 4\nabla f_i + \frac{8}{3}\nabla^2 f_i + (0)\nabla^3 f_i + \frac{14}{35}\nabla^4 f_i + ...\right]. \tag{4.99}$$

Retaining terms up to $\nabla^3 f_i$, we obtain the method

$$y_{i+1} = y_{i-3} + h\left[4f_i - 4\nabla f_i + \frac{8}{3}\nabla^2 f_i + (0)\nabla^3 f_i\right]$$

$$= y_{i-3} + h\left[4f_i - 4(f_i - f_{i-1}) + \frac{8}{3}(f_i - 2f_{i-1} + f_{i-2}\right]$$

$$= y_{i-3} + \frac{4h}{3}[2f_i - f_{i-1} + 2f_{i-2}]$$

The error term is given by

$$\text{T.E.} = \frac{14}{45} h^5 f^{(4)}(\xi) = \frac{14}{45} h^5 y^{(5)}(\xi).$$

Therefore, the method is of fourth order.

Example 4.14 *Using the Adams-Bashforth predictor-corrector equations, evaluate* $y(1.4)$, *if* y *satisfies*

$$\frac{dy}{dx} + \frac{y}{x} = \frac{1}{x^2}$$

and $y(1) = 1$, $y(1.1) = 0.996$, $y(1.2) = 0.986$, $y(1.3) = 0.972$. (*A.U. Nov./Dec. 2006*)

Solution The Adams-Bashforth predictor-corrector method is given by

Predictor P: Adams-Bashforth method of fourth order.

$$y_{i+1}^{(p)} = y_i + \frac{h}{24}[55 f_i - 59 f_{i-1} + 37 f_{i-2} - 9 f_{i-3}].$$

The method requires the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}.

Corrector C: Adams-Moulton method of fourth order.

$$y_{i+1}^{(c)} = y_i + \frac{h}{24}[9 f(x_{i+1}, y_{i+1}^{(p)}) + 19 f_i - 5 f_{i-1} + f_{i-2}]$$

The method requires the starting values y_i, y_{i-1}, y_{i-2}.

The combination requires the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}. That is, we require the values y_0, y_1, y_2, y_3. With $h = 0.1$, we are given the values

$$y(1) = 1,\ y(1.1) = 0.996,\ y(1.2) = 0.986,\ y(1.3) = 0.972.$$

We have $\quad f(x, y) = \dfrac{1}{x^2} - \dfrac{y}{x}.$

Predictor application

For $i = 3$, we obtain

$$y_4^{(0)} = y_4^{(p)} = y_3 + \frac{h}{24}[55 f_3 - 59 f_2 + 37 f_1 - 9 f_0]$$

We have
$$f_0 = f(x_0, y_0) = f(1, 1) = 1 - 1 = 0,$$
$$f_1 = f(x_1, y_1) = f(1.1, 0.996) = -\,0.079008,$$
$$f_2 = f(x_2, y_2) = f(1.2, 0.986) = -\,0.127222,$$
$$f_3 = f(x_3, y_3) = f(1.3, 0.972) = -\,0.155976.$$

$$y_4^{(0)} = 0.972 + \frac{0.1}{24}[55(-0.155976) - 59(-0.127222) + 37(-0.079008) - 9(0)]$$
$$= 0.955351.$$

Corrector application

Now, $f(x_4, y_4^{(0)}) = f(1.4, 0.955351) = -0.172189.$

First iteration

$$y_4^{(1)} = y_4^{(c)} = y_3 + \frac{h}{24}[9f(x_4, y_4^{(0)}) + 19f_3 - 5f_2 + f_1]$$

$$= 0.972 + \frac{0.1}{24}[9(-0.172189) + 19(-0.155976) - 5(-0.127222) + (-0.079008)] = 0.955516.$$

Second iteration

$$f(x_4, y_4^{(1)}) = f(1.4, 0.955516) = -0.172307.$$

$$y_4^{(2)} = y_3 + \frac{h}{24}[9f(x_4, y_4^{(1)}) + 19f_3 - 5f_2 + f_1]$$

$$= 0.972 + \frac{0.1}{24}[9(-0.172307) + 19(-0.155976) - 5(-0.127222) + (-0.079008)] = 0.955512.$$

Now, $|\, y_4^{(2)} - y_4^{(1)} \,| = |\, 0.955512 - 0.955516 \,| = 0.000004.$

Therefore, $y(1.4) = 0.955512$. The result is correct to five decimal places.

Example 4.15 *Given* $y' = x^3 + y$, $y(0) = 2$, *the values* $y(0.2) = 2.073$, $y(0.4) = 2.452$, *and* $y(0.6) = 3.023$ *are got by Runge-Kutta method of fourth order. Find* $y(0.8)$ *by Milne's predictor-corrector method taking* $h = 0.2$. (*A.U. April/May 2004*)

Solution Milne's predictor-corrector method is given by

Predictor P: Adams-Bashforth method of fourth order.

$$y_{i+1}^{(p)} = y_{i-3} + \frac{4h}{3}[2f_i - f_{i-1} + 2f_{i-2}].$$

Corrector C: Milne-Simpson's method of fourth order.

$$y_{i+1}^{(c)} = y_{i-1} + \frac{h}{3}[f(x_{i+1}, y_{i+1}^{(p)}) + 4f_i + f_{i-1}].$$

The method requires the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}. That is, we require the values y_0, y_1, y_2, y_3. Initial condition gives the value y_0.

We are given that

$$f(x, y) = x^3 + y,\ x_0 = 0,\ y_0 = 2,\ y(0.2) = y_1 = 2.073,$$

$$y(0.4) = y_2 = 2.452,\ y(0.6) = y_3 = 3.023.$$

Predictor application

For i = 3, we obtain

$$y_4^{(0)} = y_4^{(p)} = y_0 + \frac{4(0.2)}{3}[2f_3 - f_2 + 2f_1].$$

We have $f_0 = f(x_0, y_0) = f(0, 2) = 2,$

$f_1 = f(x_1, y_1) = f(0.2, 2.073) = 2.081,$

$f_2 = f(x_2, y_2) = f(0.4, 2.452) = 2.516,$

$f_3 = f(x_3, y_3) = f(0.6, 3.023) = 3.239.$

$$y_4^{(0)} = 2 + \frac{0.8}{3}[2(3.239) - 2.516 + 2(2.081)] = 4.1664.$$

Corrector application

First iteration For i = 3, we get

$$y_4^{(1)} = y_2 + \frac{0.2}{3}[f(x_4, y_4^{(0)}) + 4f_3 + f_2]$$

Now, $f(x_4, y_4^{(0)}) = f(0.8, 4.1664) = 4.6784.$

$$y_4^{(1)} = 2.452 + \frac{0.2}{3}[4.6784 + 4(3.239) + 2.516] = 3.79536.$$

Second iteration

$$y_4^{(2)} = y_2 + \frac{0.2}{3}[f(x_4, y_4^{(1)}) + 4f_3 + f_2]$$

Now, $f(x_4, y_4^{(1)}) = f(0.8, 4.6784) = 4.30736.$

$$y_4^{(2)} = 2.452 + \frac{0.2}{3}[4.30736 + 4(3.239) + 2.516] = 3.770624.$$

We have $| y_4^{(2)} - y_4^{(1)} | = | 3.770624 - 3.79536 | = 0.024736.$

The result is accurate to one decimal place.

Third iteration

$$y_4^{(3)} = y_2 + \frac{0.2}{3}[f(x_4, y_4^{(2)}) + 4f_3 + f_2]$$

Now, $f(x_4, y_4^{(2)}) = f(0.8, 3.770624) = 4.282624.$

$$y_4^{(3)} = 2.452 + \frac{0.2}{3}[4.282624 + 4(3.239) + 2.516] = 3.768975.$$

We have $| y_4^{(3)} - y_4^{(2)} | = | 3.768975 - 3.770624 | = 0.001649.$

The result is accurate to two decimal places.

Fourth iteration

$$y_4^{(4)} = y_2 + \frac{0.2}{3}[f(x_4, y_4^{(3)}) + 4f_3 + f_2]$$

Now, $\quad f(x_4, y_4^{(3)}) = f(0.8, 3.76897) = 4.280975.$

$$y_4^{(4)} = 2.452 + \frac{0.2}{3}\ [4.280975 + 4(3.239) + 2.516] = 3.768865.$$

We have $\mid y_4^{(4)} - y_4^{(3)} \mid = \mid 3.768865 - 3.768975 \mid = 0.000100.$

The result is accurate to three decimal places.

The required result can be taken as $y(0.8) = 3.7689$.

Example 4.16 *Using Milne's predictor-corrector method, find* $y(0.4)$ *for the initial value problem*

$$y' = x^2 + y^2,\ y(0) = 1,\ \text{with } h = 0.1.$$

Calculate all the required initial values by Euler's method. The result is to be accurate to three decimal places.

Solution Milne's predictor-corrector method is given by

Predictor P: Adams-Bashforth method of fourth order.

$$y_{i+1}^{(p)} = y_{i-3} + \frac{4h}{3}[2f_i - f_{i-1} + 2f_{i-2}].$$

Corrector C: Milne-Simpson's method of fourth order.

$$y_{i+1}^{(c)} = y_{i-1} + \frac{h}{3}[f(x_{i+1}, y_{i+1}^{(p)}) + 4f_i + f_{i-1}].$$

The method requires the starting values y_i, y_{i-1}, y_{i-2} and y_{i-3}. That is, we require the values y_0, y_1, y_2, y_3. Initial condition gives the value y_0.

We are given that

$$f(x, y) = x^2 + y^2,\ x_0 = 0,\ y_0 = 1.$$

Euler's method gives

$$y_{i+1} = y_i + hf(x_i, y_i) = y_i + 0.1(x_i^2 + y_i^2).$$

With $x_0 = 0$, $y_0 = 1$, we get

$$y_1 = y_0 + 0.1\ (x_0^2 + y_0^2) = 1.0 + 0.1\ (0 + 1.0) = 1.1.$$

$$y_2 = y_1 + 0.1\ (x_1^2 + y_1^2) = 1.1 + 0.1\ (0.01 + 1.21) = 1.222.$$

$$y_3 = y_2 + 0.1\ (x_2^2 + y_2^2) = 1.222 + 0.1[0.04 + (1.222)^2] = 1.375328.$$

Predictor application

For i = 3, we obtain

$$y_4^{(0)} = y_4^{(p)} = y_0 + \frac{4(0.1)}{3}[2f_3 - f_2 + 2f_1]$$

We have $f_1 = f(x_1, y_1) = f(0.1, 1.1) = 1.22,$

$f_2 = f(x_2, y_2) = f(0.1, 1.222) = 1.533284,$

$f_3 = f(x_3, y_3) = f(0.3, 1.375328) = 1.981527.$

$$y_4^{(0)} = 1.0 + \frac{0.4}{3}[2(1.981527) - 1.533284 + 2(1.22)] = 1.649303.$$

Corrector application

First iteration For i = 3, we get

$$y_4^{(1)} = y_2 + \frac{0.1}{3}[f(x_4, y_4^{(0)}) + 4f_3 + f_2]$$

Now, $f(x_4, y_4^{(0)}) = f(0.4, 1.649303) = 2.880200.$

$$y_4^{(1)} = 1.222 + \frac{0.1}{3}[2.880200 + 4(1.981527) + 1.533284] = 1.633320.$$

Second iteration

$$y_4^{(2)} = y_2 + \frac{0.1}{3}[f(x_4, y_4^{(1)}) + 4f_3 + f_2]$$

Now, $f(x_4, y_4^{(1)}) = f(0.4, 1.633320) = 2.827734.$

$$y_4^{(2)} = 1.222 + \frac{0.1}{3}[2.827734 + 4(1.981527) + 1.533284] = 1.631571.$$

We have $|\ y_4^{(2)} - y_4^{(1)}\ | = |\ 1.631571 - 1.633320\ | = 0.001749.$

The result is accurate to two decimal places.

Third iteration

$$y_4^{(3)} = y_2 + \frac{0.1}{3}[f(x_4, y_4^{(2)}) + 4f_3 + f_2]$$

Now, $f(x_4, y_4^{(2)}) = f(0.4, 1.631571) = 2.822024.$

$$y_4^{(3)} = 1.222 + \frac{0.1}{3}[2.822024 + 4(1.981527) + 1.533284] = 1.631381.$$

We have $|\ y_4^{(3)} - y_4^{(2)}\ | = |\ 1.631381 - 1.631571\ | = 0.00019.$

The result is accurate to three decimal places.

The required result can be taken as $y(0.4) \approx 1.63138$.

5

Boundary Value Problems in Ordinary Differential Equations and Initial and Boundary Value Problems in Partial Differential Equations

5.1 INTRODUCTION

Boundary value problems are of great importance in science and engineering. In this chapter, we shall discuss the numerical solution of the following problems:

(*a*) Boundary value problems in ordinary differential equations.

(*b*) Boundary value problems governed by linear second order partial differential equations. We shall discuss the solution of the *Laplace equation* $u_{xx} + u_{yy} = 0$ and the *Poisson equation* $u_{xx} + u_{yy} = G(x, y)$.

(*c*) Initial boundary value problems governed by linear second order partial differential equations. We shall discuss the solution of the *heat equation* $u_t = c^2 u_{xx}$ and the *wave equation* $u_{tt} = c^2 u_{xx}$ under the given initial and boundary conditions.

5.2 BOUNDARY VALUE PROBLEMS GOVERNED BY SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS

A general second order ordinary differential equation is given by

$$y'' = f(x, y, y'), \quad x \in [a, b]. \tag{5.1}$$

Since the ordinary differential equation is of second order, we need to prescribe two suitable conditions to obtain a unique solution of the problem. If the conditions are prescribed at the end points $x = a$ and $x = b$, then it is called a *two-point boundary value problem.* For our discussion in this chapter, we shall consider only the linear second order ordinary differential equation

$$a_0(x)\, y'' + a_1(x)\, y' + a_2(x)\, y = d(x), \quad x \in [a, b] \tag{5.2}$$

or, in the form

$$y'' + p(x)\, y' + q(x)\, y = r(x), \quad x \in [a, b]. \tag{5.3}$$

We shall assume that the solution of Eq.(5.3) exists and is unique. This implies that $a_0(x)$, $a_1(x)$, $a_2(x)$ and $d(x)$, or $p(x)$, $q(x)$ and $r(x)$ are continuous for all $x \in [a, b]$.

The two conditions required to solve Eq.(5.2) or Eq.(5.3), can be prescribed in the following three ways:

(*i*) *Boundary conditions of first kind* The dependent variable $y(x)$ is prescribed at the end points $x = a$ and $x = b$.

$$y(a) = A, \; y(b) = B. \tag{5.4}$$

(*ii*) *Boundary conditions of second kind* The normal derivative of $y(x)$, (slope of the solution curve) is prescribed at the end points $x = a$ and $x = b$.

$$y'(a) = A, \; y'(b) = B. \tag{5.5}$$

(*iii*) *Boundary conditions of third kind or mixed boundary conditions*

$$\begin{aligned} a_0\, y(a) - a_1\, y'(a) &= A, \\ b_0 y(b) + b_1\, y'(b) &= B, \end{aligned} \tag{5.6}$$

where a_0, a_1, b_0, b_1, A and B are constants such that

$$a_0 a_1 \ge 0, \; |\, a_0 \,| + |\, a_1 \,| \ne 0, \; b_0 b_1 \ge 0, \; |\, b_0 \,| + |\, b_1 \,| \ne 0, \quad |\, a_0 \,| + |\, b_0 \,| \ne 0.$$

We shall consider the solution of Eq.(5.2) or Eq.(5.3) under the boundary conditions of first kind only, that is, we shall consider the solution of the boundary value problem

$$\begin{aligned} y'' + p(x)\, y' + q(x)\, y &= r(x), \quad x \in [a, b] \\ y(a) = A, \quad y(b) &= B. \end{aligned} \tag{5.7}$$

Finite difference method Subdivide the interval $[a, b]$ into n equal sub-intervals. The length of the sub-interval is called the *step length*. We denote the step length by Δx or h. Therefore,

$$\Delta x = h = \frac{b - a}{n}, \text{ or } b = a + nh.$$

The points $a = x_0$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, ..., $x_i = x_0 + ih$, ..., $x_n = x_0 + nh = b$, are called the *nodes* or *nodal points* or *lattice points* (Fig. 5.1).

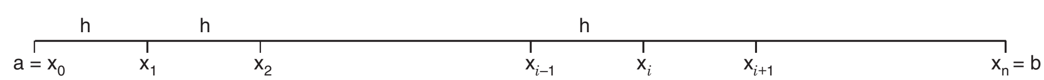

Fig. 5.1 Nodes.

We denote the numerical solution at any point x_i by y_i and the exact solution by $y(x_i)$.

In Chapter 3, we have derived the following approximations to the derivatives.

Approximation to $y'(x_i)$ at the point $x = x_i$

(*i*) Forward difference approximation of first order or $O(h)$ approximation:

$$y'(x_i) \approx \frac{1}{h}[y(x_{i+1}) - y(x_i)], \quad \text{or} \quad y'_i = \frac{1}{h}\,[y_{i+1} - y_i]. \tag{5.8}$$

(*ii*) Backward difference approximation of first order or $O(h)$ approximation:

$$y'(x_i) \approx \frac{1}{h}[y(x_i) - y(x_{i-1})], \quad \text{or} \quad y'_i = \frac{1}{h}[y_i - y_{i-1}]. \tag{5.9}$$

(*iii*) Central difference approximation of second order or $O(h^2)$ approximation:

$$y'(x_i) \approx \frac{1}{2h}[y(x_{i+1}) - y(x_{i-1})], \text{ or } y'_i = \frac{1}{2h}[y_{i+1} - y_{i-1}]. \tag{5.10}$$

Approximation to $y''(x_i)$ at the point $x = x_i$

Central difference approximation of second order or $O(h^2)$ approximation:

$$y''(x_i) \approx \frac{1}{h^2}[y(x_{i+1}) - 2y(x_i) + y(x_{i-1})],$$

or

$$y''_i = \frac{1}{h^2}[y_{i+1} - 2y_i + y_{i-1}]. \tag{5.11}$$

Applying the differential equation (5.3) at the nodal point $x = x_i$, we obtain

$$y''(x_i) + p(x_i)\, y'(x_i) + q(x_i)\, y(x_i) = r(x_i). \tag{5.12}$$

Since $y(a) = y(x_0) = A$ and $y(b) = y(x_n) = B$ are prescribed, we need to determine the numerical solutions at the $n - 1$ nodal points $x_1, x_2, ..., x_i, ..., x_{n-1}$.

Now, $y'(x_i)$ is approximated by one of the approximations given in Eqs. (5.8), (5.9), (5.10) and $y''(x_i)$ is approximated by the approximation given in Eq.(5.11). Since the approximations (5.10) and (5.11) are both of second order, the approximation to the differential equation is of second order. However, if $y'(x_i)$ is approximated by (5.8) or (5.9), which are of first order, then the approximation to the differential equation is only of first order. But, in many practical problems, particularly in Fluid Mechanics, approximations (5.8), (5.9) give better results (non-oscillatory solutions) than the central difference approximation (5.10).

Using the approximations (5.10) and (5.11) in Eq.(5.12), we obtain

$$\frac{1}{h^2}[y_{i+1} - 2y_i + y_{i-1}] + \frac{p(x_i)}{2h}[y_{i+1} - y_{i-1}] + q(x_i)\, y_i = r_i$$

or

$$2[y_{i+1} - 2y_i + y_{i-1}] + h\, p(x_i)\, [y_{i+1} - y_{i-1}] + 2h^2\, q(x_i)\, y_i = 2h^2\, r_i\, .$$

Collecting the coefficients, we can write the equation as

$$a_i\, y_{i-1} + b_i\, y_i + c_i\, y_{i+1} = d_i, \quad i = 1, 2, \ldots, n - 1 \tag{5.13}$$

where $a_i = 2 - h\, p(x_i)$, $b_i = -4 + 2h^2\, q(x_i)$, $c_i = 2 + h\, p(x_i)$, $d_i = 2h^2 r(x_i)$.

Let us now apply the method at the nodal points. We have the following equations.

At $x = x_1$, or $i = 1$:

$$a_1 y_0 + b_1 y_1 + c_1 y_2 = d_1, \quad \text{or} \quad b_1 y_1 + c_1 y_2 = d_1 - a_1 A = d_1^*. \tag{5.14}$$

At $x = x_i$, $i = 2, 3, \ldots, n - 2$:

$$a_i y_{i-1} + b_i y_i + c_i y_{i+1} = d_i \tag{5.15}$$

At $x = x_{n-1}$, or $i = n - 1$:

$$a_{n-1} y_{n-2} + b_{n-1} y_{n-1} + c_{n-1} y_n = d_{n-1}, \text{ or } a_{n-1} y_{n-2} + b_{n-1} y_{n-1} = d_{n-1} - c_{n-1} B = d^*_{n-1}. \quad (5.16)$$

Eqs.(5.14), (5.15), (5.16) give rise to a system of $(n - 1) \times (n - 1)$ equations $\mathbf{Ay = d}$ for the unknowns $y_1, y_2, ..., y_i, ..., y_{n-1}$, where $\mathbf{A}$ is the coefficient matrix and

$$\mathbf{y} = [y_1, y_2, ..., y_i, ..., y_{n-1}]^T, \quad \mathbf{d} = [d^*_1, d_2, ..., d_i, ..., d_{n-2}, d^*_{n-1}]^T.$$

It is interesting to study the structure of the coefficient matrix **A.** Consider the case when the interval $[a, b]$ is subdivided into $n = 10$ parts. Then, we have 9 unknowns, $y_1, y_2, ...,$ y_9, and the coefficient matrix **A** is as given below.

Remark 1 *Do you recognize the structure of* **A?** It is a *tri-diagonal system* of algebraic equations. Therefore, the numerical solution of Eq.(5.2) or Eq.(5.3) by finite differences gives rise to a tri-diagonal system of algebraic equations, whose solution can be obtained by using the Gauss elimination method or the *Thomas algorithm.* Tri-diagonal system of algebraic equations is the easiest to solve. In fact, even if the system is very large, its solution can be obtained in a few minutes on a modern desk top *PC*.

$$\mathbf{A} = \begin{bmatrix} b_1 & c_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_4 & b_4 & c_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_5 & b_5 & c_5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a_6 & b_6 & c_6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a_7 & b_7 & c_7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a_8 & b_8 & c_8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_9 & c_9 \end{bmatrix}$$

Remark 2 *Does the system of equations* (5.13) *always converge*? We have the following sufficient condition: *If the system of equations* (5.13) *is diagonally dominant, then it always converges.* Using the expressions for a_i, b_i, c_i, we can try to find the bound for h for which this condition is satisfied.

Example 5.1 *Derive the difference equations for the solution of the boundary value problem*

$$y'' + p(x)\, y' + q(x)\, y = r(x), \qquad x \in [a, b]$$

$$y(a) = A,\ y(b) = B$$

using central difference approximation for y'' and forward difference approximation for y'.

Solution Using the approximations

$$y_i'' = \frac{1}{h^2} [y_{i+1} - 2y_i + y_{i-1}], \qquad y_i' = \frac{1}{h} [y_{i+1} - y_i]$$

in the differential equation, we obtain

$$\frac{1}{h^2} [y_{i+1} - 2y_i + y_{i-1}] + \frac{p(x_i)}{h} [y_{i+1} - y_i] + q(x_i) y_i = r(x_i)$$

or $\quad [y_{i+1} - 2y_i + y_{i-1}] + h\,p(x_i)\,[y_{i+1} - y_i] + h^2 q(x_i)\,y_i = h^2 r_i$

or $\quad y_{i-1} + b_i y_i + c_i y_{i+1} = d_i, \qquad i = 1, 2, \ldots, n-1$

where $\quad b_i = -2 - h\,p(x_i) + h^2 q(x_i), \quad c_i = 1 + h\,p(x_i),\ d_i = h^2 r_i.$

The system again produces a tri-diagonal system of equations.

Example 5.2 *Derive the difference equations for the solution of the boundary value problem*

$$y'' + p(x)\,y' + q(x)\,y = r(x), \quad x \in [a, b]$$

$$y(a) = A, \quad y(b) = B$$

using central difference approximation for y'' and backward difference approximation for y'.

Solution Using the approximations

$$y_i'' = \frac{1}{h^2}[y_{i+1} - 2y_i + y_{i-1}], \qquad y_i' = \frac{1}{h}[y_i - y_{i-1}]$$

in the differential equation, we obtain

$$\frac{1}{h^2}[y_{i+1} - 2y_i + y_{i-1}] + \frac{p(x_i)}{h}[y_i - y_{i-1}] + q(x_i)\,y_i = r(x_i)$$

or $\quad [y_{i+1} - 2y_i + y_{i-1}] + h\,p(x_i)\,[y_i - y_{i-1}] + h^2 q(x_i) y_i = h^2 r_i$

or $\quad a_i y_{i-1} + b_i y_i + y_{i+1} = d_i, \quad i = 1, 2, \ldots, n-1$

where $\quad a_i = 1 - h\,p(x_i),\ b_i = -2 + h\,p(x_i) + h^2 q(x_i),\ d_i = h^2 r_i.$

The system again produces a tri-diagonal system of equations.

Example 5.3 *Solve the boundary value problem* $x\,y'' + y = 0$, $y(1) = 1$, $y(2) = 2$ *by second order finite difference method with* $h = 0.25$.

Solution We have $h = 0.25$ and $n = \dfrac{b-a}{h} = \dfrac{2-1}{0.25} = 4.$

We have five nodal points $x_0 = 1.0$, $x_1 = 1.25$, $x_2 = 1.5$, $x_3 = 1.75$, $x_4 = 2.0$.

We are given the data values $y(x_0) = y_0 = y(1) = 1$, $y(x_4) = y_4 = y(2) = 2$.

We are to determine the approximations for $y(1.25)$, $y(1.5)$, $y(1.75)$. Using the central difference approximation for y_i'', we get

$$\frac{x_i}{h^2}[y_{i+1} - 2y_i + y_{i-1}] + y_i = 0, \quad \text{or} \quad 16x_i\,y_{i-1} + (1 - 32x_i)\,y_i + 16x_i\,y_{i+1} = 0.$$

We have the following difference equations.

For $i = 1$, $x_1 = 1.25$, $y_0 = 1.0$: $\quad 20y_0 - 39y_1 + 20y_2 = 0$ or $-39y_1 + 20y_2 = -20$

For $i = 2$, $x_2 = 1.5$: $\quad 24y_1 - 47y_2 + 24y_3 = 0.$

For $i = 3$, $x_3 = 1.75$, $y_4 = 2.0$: $\quad 28y_2 - 55y_3 + 28y_4 = 0$ or $28y_2 - 55y_3 = -56.$

We have the following system of equations

$$\begin{bmatrix} -39 & 20 & 0 \\ 24 & -47 & 24 \\ 0 & 28 & -55 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} -20 \\ 0 \\ -56 \end{bmatrix}.$$

We can solve this system using Gauss elimination. We obtain

$$\left[\begin{array}{ccc|c} -39 & 20 & 0 & -20 \\ 24 & -47 & 24 & 0 \\ 0 & 28 & -55 & -56 \end{array}\right], \frac{R_1}{-39}, \left[\begin{array}{ccc|c} 1 & -20/39 & 0 & 20/39 \\ 24 & -47 & 24 & 0 \\ 0 & 28 & -55 & -56 \end{array}\right], R_2 - 24R_1,$$

$$\left[\begin{array}{ccc|c} 1 & -20/39 & 0 & 20/39 \\ 0 & -1353/39 & 24 & -480/39 \\ 0 & 28 & -55 & -56 \end{array}\right], \frac{R_2}{(-1353/39)}, \left[\begin{array}{ccc|c} 1 & -20/39 & 0 & 20/39 \\ 0 & 1 & -936/1353 & 480/1353 \\ 0 & 28 & -55 & -56 \end{array}\right],$$

$$R_3 - 28R_2, \left[\begin{array}{ccc|c} 1 & -20/39 & 0 & 20/39 \\ 0 & 1 & -936/1353 & 480/1353 \\ 0 & 0 & -48207/1353 & -89208/1353 \end{array}\right]$$

From the last equation, we get $y_3 = \dfrac{89208}{48207} = 1.85052.$

Back substitution gives $y_2 = \dfrac{480}{1353} + \dfrac{936}{1353}(1.85052) = 1.63495,$

$$y_1 = \frac{20}{39}(1 + 1.63495) = 1.35126.$$

Example 5.4 *Using the second order finite difference method, find* $y(0.25)$, $y(0.5)$, $y(0.75)$ *satisfying the differential equation* $y'' - y = x$ *and subject to the conditions* $y(0) = 0$, $y(1) = 2$.

Solution We have $h = 0.25$ and $n = \dfrac{b-a}{h} = \dfrac{1-0}{0.25} = 4.$

We have five nodal points $x_0 = 0.0$, $x_1 = 0.25$, $x_2 = 0.5$, $x_3 = 0.75$, $x_4 = 1.0$.

We are given the data values $y(x_0) = y_0 = y(0) = 0$, $y(x_4) = y_4 = y(1) = 2$.

We are to determine the approximations for $y(0.25)$, $y(0.5)$, $y(0.75)$. Using the central difference approximation for y_i'', we get

$$\frac{1}{h^2}[y_{i+1} - 2y_i + y_{i-1}] - y_i = x_i, \text{ or } 16y_{i-1} - 33y_i + 16y_{i+1} = x_i.$$

We have the following difference equations.

For $i = 1$, $x_1 = 0.25$, $y_0 = 0.0$: $16y_0 - 33y_1 + 16y_2 = 0.25$ or $-33y_1 + 16y_2 = 0.25$,

For $i = 2$, $x_2 = 0.5$: $16y_1 - 33y_2 + 16y_3 = 0.5$,

For $i = 3$, $x_3 = 0.75$, $y_4 = 2.0$: $16y_2 - 33y_3 + 16y_4 = 0.75$ or $16y_2 - 33y_3 = -31.25$.

We have the following system of equations

$$\begin{bmatrix} -33 & 16 & 0 \\ 16 & -33 & 16 \\ 0 & 16 & -33 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 0.25 \\ 0.5 \\ -31.25 \end{bmatrix}.$$

We can solve this system using Gauss elimination. We obtain

$$\left[\begin{array}{ccc|c} -33 & 16 & 0 & 0.25 \\ 16 & -33 & 16 & 0.5 \\ 0 & 16 & -33 & -31.25 \end{array}\right], \frac{R_1}{-33}, \left[\begin{array}{ccc|c} 1 & -0.48485 & 0 & -0.007576 \\ 16 & -33 & 16 & 0.5 \\ 0 & 16 & -33 & -56 \end{array}\right], \; R_2 - 16R_1,$$

$$\left[\begin{array}{ccc|c} 1 & -0.48485 & 0 & -0.007576 \\ 0 & -25.2424 & 16 & 0.621216 \\ 0 & 16 & -33 & -31.25 \end{array}\right], \frac{R_2}{(-25.2424)}, \left[\begin{array}{ccc|c} 1 & -0.48485 & 0 & -0.007576 \\ 0 & 1 & -0.63385 & -0.02461 \\ 0 & 16 & -33 & -31.25 \end{array}\right],$$

$$R_3 - 16R_2, \; \left[\begin{array}{ccc|c} 1 & -0.48485 & 0 & -0.007576 \\ 0 & 1 & -0.63385 & -0.02461 \\ 0 & 0 & -22.8584 & -30.85624 \end{array}\right].$$

From the last equation, we get $\quad y_3 = \dfrac{30.85624}{22.8584} = 1.34989.$

Back substitution gives

$$y_2 = -0.02461 + 0.63385(1.34989) = 0.83102,$$

$$y_1 = -0.007576 + 0.48485(0.83102) = 0.39534.$$

Example 5.5 *Solve the boundary value problem* $y'' + 5y' + 4y = 1$, $y(0) = 0$, $y(1) = 0$ *by finite difference method. Use central difference approximations with* $h = 0.25$. *If the exact solution is*

$$y(x) = Ae^{-x} + Be^{-4x} + 0.25, \text{ where } A = \frac{e^{-3} - e}{4(1 - e^{-3})}, B = -0.25 - A$$

find the magnitude of the error and percentage relative error at $x = 0.5$.

Solution We have $h = 0.25$ and $n = \dfrac{b-a}{h} = \dfrac{1-0}{0.25} = 4.$

We have five nodal points $\qquad x_0 = 0.0,\ x_1 = 0.25,\ x_2 = 0.5,\ x_3 = 0.75,\ x_4 = 1.0.$

We are given the data values $y(x_0) = y_0 = y(0) = 0$, $y(x_4) = y_4 = y(1) = 0$.

We are to determine the approximations for $y(0.25)$, $y(0.5)$, $y(0.75)$. Using the central difference approximations, we get

$$\frac{1}{h^2}[y_{i+1} - 2y_i + y_{i-1}] + \frac{5}{2h}(y_{i+1} - y_{i-1}) + 4y_i = 1,$$

or $$16[y_{i+1} - 2y_i + y_{i-1}] + 10(y_{i+1} - y_{i-1}) + 4y_i = 1, \quad \text{or} \quad 6y_{i-1} - 28y_i + 26y_{i+1} = 1.$$

We have the following difference equations.

For $i = 1$, $x_1 = 0.25$, $y_0 = 0.0$: $6y_0 - 28y_1 + 26y_2 = 1$ or $-28y_1 + 26y_2 = 1$.

For $i = 2$, $x_2 = 0.5$: $6y_1 - 28y_2 + 26y_3 = 1$.

For $i = 3$, $x_3 = 0.75$, $y_4 = 0$: $6y_2 - 28y_3 + 26y_4 = 1$ or $6y_2 - 28y_3 = 1$.

We have the following system of equations

$$\begin{bmatrix} -28 & 26 & 0 \\ 6 & -28 & 26 \\ 0 & 6 & -28 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

We can solve this system using Gauss elimination. We obtain

$$\left[\begin{array}{ccc|c} -28 & 26 & 0 & 1 \\ 6 & -28 & 26 & 1 \\ 0 & 6 & -28 & 1 \end{array}\right], \frac{R_1}{-28}, \left[\begin{array}{ccc|c} 1 & -0.92857 & 0 & -0.03571 \\ 6 & -28 & 26 & 1 \\ 0 & 6 & -28 & 1 \end{array}\right], \; R_2 - 6R_1$$

$$\left[\begin{array}{ccc|c} 1 & -0.92857 & 0 & -0.03571 \\ 0 & -22.42858 & 26 & 1.21426 \\ 0 & 6 & -28 & 1 \end{array}\right], \frac{R_2}{(-22.42858)}, \left[\begin{array}{ccc|c} 1 & -0.92857 & 0 & -0.03571 \\ 0 & 1 & -1.15924 & -0.05414 \\ 0 & 6 & -28 & 1 \end{array}\right]$$

$$R_3 - 6R_2, \left[\begin{array}{ccc|c} 1 & -0.92857 & 0 & -0.03571 \\ 0 & 1 & -1.15924 & -0.05414 \\ 0 & 0 & -21.04456 & 1.32484 \end{array}\right].$$

From the last equation, we get $y_3 = \dfrac{1.32484}{-21.04456} = -0.06295.$

Back substitution gives

$$y_2 = -0.05414 - 1.15924(0.06295) = -0.12711,$$

$$y_1 = -0.03571 - 0.92857(0.12711) = -0.15374.$$

We also have $A = -0.70208$, $B = 0.45208$, $y(0.5) = Ae^{-0.5} + Be^{-2} = 0.11465$.

Now, $|$ error at $x = 0.5$ $| = | y_2 - y(0.5) | = | -0.12711 + 0.11465 | = 0.01246$.

$$\text{Percentage relative error} = \frac{0.01246}{0.11465}(100) = 10.8\%.$$

Example 5.6 *Solve the boundary value problem*

$$(1 + x^2)y'' + 4xy' + 2y = 2, \quad y(0) = 0, \; y(1) = 1/2$$

by finite difference method. Use central difference approximations with $h = 1/3$.

Solution We have $h = 1/3$. The nodal points are $x_0 = 0$, $x_1 = 1/3$, $x_2 = 2/3$, $x_3 = 1$.

Using the central difference approximations, we obtain

$$\frac{1}{h^2}(1+x_i^2)[y_{i+1}-2y_i+y_{i-1}]+\frac{4x_i}{2h}(y_{i+1}-y_{i-1})+2y_i = 2$$

or $$[9(1+x_i^2)-6x_i]y_{i-1}+[2-18(1+x_i^2)]y_i+[9(1+x_i^2)+6x_i]y_{i+1} = 2.$$

We have the following difference equations.

For $i = 1$, $x_1 = 1/3$, $y_0 = 0$:

$$\left[9\left(1+\frac{1}{9}\right)-2\right]y_0+\left[2-18\left(1+\frac{1}{9}\right)\right]y_1+\left[9\left(1+\frac{1}{9}\right)+2\right]y_2 = 2$$

or $\quad - 18y_1 + 12y_2 = 2.$

For $i = 2$, $x_1 = 2/3$, $y_3 = 1/2$:

$$\left[9\left(1+\frac{4}{9}\right)-4\right]y_1+\left[2-18\left(1+\frac{4}{9}\right)\right]y_2+\left[9\left(1+\frac{4}{9}\right)+4\right]y_3 = 2$$

or $\quad 9y_1 - 24y_2 = - 6.5.$

Solving the equations

$$- 9y_1 + 6y_2 = 1,\ 9y_1 - 24y_2 = - 6.5$$

we obtain $$y_1 = \frac{15}{162} = 0.092592,\ y_2 = \frac{49.5}{162} = 0.305556.$$

REVIEW QUESTIONS

1. Write the first order difference approximations for $y'(x_i)$ based on (*i*) forward differences, (*ii*) backward differences.

Solution

(*i*) $y'(x_i) = [y_{i+1} - y_i]/(h)$, (*ii*) $y'(x_i) = [y_i - y_{i-1}]/h$, where h is the step length.

2. Write the second order difference approximations for (*i*) $y'(x_i)$, (*ii*) $y''(x_i)$ based on central differences.

Solution (*i*) $y'(x_i) = [y_{i+1} - y_{i-1}]/(2h)$, (*ii*) $y''(x_i) = [y_{i+1} - 2y_i + y_{i-1}]/h^2$,

where h is the step length.

3. Finite difference methods when applied to linear second order boundary value problems in ordinary differential equations produce a system of linear equations **Ay = b.** What is the structure of the coefficient matrix **A** ?

Solution Tridiagonal matrix.

4. What types of methods are available for the solution of linear system of algebraic equations ?

Solution (*i*) Direct methods. (*ii*) Iterative methods.

First, we classify the linear second order partial differential equation

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu + G = 0 \tag{5.17}$$

where *A, B, C, D, E, F* and *G* are functions of *x, y* or are real constants.

The partial differential equation is called a

Elliptic equation if $B^2 - AC < 0$ (5.18 *i*)

Parabolic equation if $B^2 - AC = 0$ (5.18 *ii*)

Hyperbolic equation if $B^2 - AC > 0$. (5.18 *iii*)

Remark 3 Some books write the coefficient of u_{xy} in Eq.(5.17) as *B.* Then, the condition in Eq.(5.18) changes to $B^2 - 4AC$. Note that the lower order terms do not contribute to the classification of the partial differential equation.

The simplest examples of the above equations are the following:

Parabolic equation: $u_t = c^2 u_{xx}$, (One dimensional heat equation). (5.19)

Hyperbolic equation: $u_{tt} = c^2 u_{xx}$, (One dimensional wave equation). (5.20)

Elliptic equation: $u_{xx} + u_{yy} = 0$, (Two dimensional Laplace equation). (5.21)

We can verify that

in Eq.(5.19), $A = c^2, B = 0, C = 0$ and $B^2 - AC = 0$.

in Eq.(5.20), $A = c^2, B = 0, C = -1$ and $B^2 - AC = c^2 > 0$.

in Eq.(5.21), $A = 1, B = 0, C = 1$ and $B^2 - AC = -1 < 0$.

Remark 4 *What is the importance of classification*? Classification governs the number and type of conditions that should be prescribed in order that the problem has a unique solution. For example, for the solution of the one dimensional heat equation (Eq.(5.19)), we require an initial condition to be prescribed, $u(x, 0) = f(x)$, and the conditions along the boundary lines $x = 0$, and $x = l$, where l is the length of the rod (boundary conditions), are to be prescribed.

Suppose that the one dimensional wave equation (Eq.(5.20)) represents the vibrations of an elastic string of length l. Here, $u(x, t)$ represents the displacement of the string in the vertical plane. For the solution of this equation, we require two initial conditions to be prescribed, the initial displacement $u(x, 0) = f(x)$, the initial velocity $u_t(x, 0) = g(x)$, and the conditions along the boundary lines $x = 0$ and $x = l$, (boundary conditions), are to be prescribed.

For the solution of the Laplace's equation (Eq.(5.21)), we require the boundary conditions to be prescribed on the bounding curve.

Remark 5 Elliptic equation together with the boundary conditions is called an *elliptic boundary value problem.* The boundary value problem holds in a closed domain or in an open domain which can be conformally mapped on to a closed domain. For example, Laplace's equation (Eq.(5.21)) may be solved inside, say, a rectangle, a square or a circle etc. Both the hyperbolic and parabolic equations together with their initial and boundary conditions are called *initial value problems.* Sometimes, they are also called *initial-boundary value problems*. The initial value problem holds in either an open or a semi-open domain. For example, in the case of the one dimensional heat equation (Eq.(5.19)), x varies from 0 to l and $t > 0$. In the case of the one dimensional wave equation (Eq.(5.20)), x varies from 0 to l and $t > 0$.

Example 5.7 *Classify the following partial differential equations.*

(*a*) $u_{xx} = 6u_x + 3u_y$. (*b*) $2u_{xx} + 3u_{yy} - u_x + 2u_y = 0$.

(*c*) $u_{tt} + 4u_{tx} + 4u_{xx} + 2u_x + u_t = 0$. (*d*) $u_{xx} + 2xu_{xy} + (1 - y^2)u_{yy} = 0$.

Solution

(*a*) Write the given equation as $u_{xx} - 6u_x - 3u_y = 0$. We have $A = 1$, $B = 0$, $C = 0$ and $B^2 - AC = 0$. Hence, the given partial differential equation is a parabolic equation.

(*b*) We have $A = 2$, $B = 0$, $C = 3$ and $B^2 - AC = -6 < 0$. Hence, the given partial differential equation is an elliptic equation.

(*c*) We have $A = 1$, $B = 2$, $C = 4$ and $B^2 - AC = 0$. Hence, the given partial differential equation is a parabolic equation.

(*d*) We have $A = 1$, $B = x$, $C = 1 - y^2$ and $B^2 - AC = x^2 - (1 - y^2) = x^2 + y^2 - 1$. Hence, if $x^2 + y^2 - 1 > 0$, that is, outside the unit circle $x^2 + y^2 = 1$, the given partial differential equation is an hyperbolic equation. If $x^2 + y^2 - 1 = 0$, that is, on the unit circle $x^2 + y^2 = 1$, the given partial differential equation is a parabolic equation. If $x^2 + y^2 - 1 < 0$, that is, inside the unit circle $x^2 + y^2 = 1$, the given partial differential equation is an elliptic equation (see Fig. 5.2).

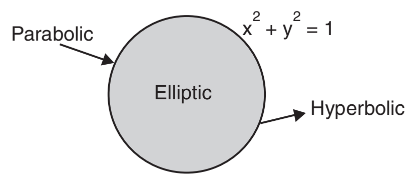

Fig. 5.2. Example 5.7.

EXERCISE 5.2

Classify the following partial differential equations.

1. $u_{xx} + 4u_{yy} = u_x + 2u_y = 0$.

2. $u_{xx} - u_{yy} + 3u_x + 4u_y = 0$.

3. $u_{xx} + 4xu_{xy} + (1 - 4y^2)u_{yy} = 0$.

4. $u_{tt} + (5 + 2x^2)u_{xt} + (1 + x^2)(4 + x^2)u_{xx} = 0$.

5. $u_{xx} + 4u_{xy} + (x^2 + 4y^2)u_{yy} = x^2 + y^2$.

5.4 FINITE DIFFERENCE METHODS FOR LAPLACE AND POISSON EQUATIONS

In this section, we consider the solution of the following boundary value problems governed by the given partial differential equations along with suitable boundary conditions.

(*a*) *Laplace's equation:* $u_{xx} + u_{yy} = \nabla^2 u = 0$, with $u(x, y)$ prescribed on the boundary, that is, $u(x, y) = f(x, y)$ on the boundary.

(*b*) *Poisson's equation:* $u_{xx} + u_{yy} = \nabla^2 u = G(x, y)$, with $u(x, y)$ prescribed on the boundary, that is, $u(x, y) = g(x, y)$ on the boundary.

In both the problems, the boundary conditions are called *Dirichlet boundary conditions* and the boundary value problem is called a *Dirichlet boundary value problem.*

Finite difference method We have a two dimensional domain $(x, y) \in R$. We superimpose on this domain R, a rectangular network or mesh of lines with step lengths h and k respectively, parallel to the x- and y-axis. The mesh of lines is called a grid. The points of intersection of the mesh lines are called *nodes* or *grid points* or *mesh points.* The grid points are given by (x_i, y_j), (see Figs. 5.3 *a*, *b*), where the mesh lines are defined by

$$x_i = ih,\ i = 0, 1, 2, ...;\ y_j = jk,\ j = 0, 1, 2, ...$$

If $h = k$, then we have a uniform mesh. Denote the numerical solution at (x_i, y_j) by $u_{i,j}$.

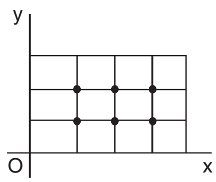

Fig. 5.3a. Nodes in a rectangle.

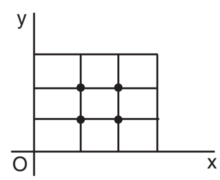

Fig. 5.3b. Nodes in a square.

At the nodes, the partial derivatives in the differential equation are replaced by suitable difference approximations. That is, the partial differential equation is approximated by a difference equation at each nodal point. This procedure is called *discretization* of the partial differential equation. We use the following central difference approximations.

$$(u_x)_{i,j} = \frac{1}{2h}(u_{i+1,j} - u_{i-1,j}), \quad (u_y)_{i,j} = \frac{1}{2k}(u_{i,j+1} - u_{i,j-1}),$$

$$(u_{xx})_{i,j} = \frac{1}{h^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}), \quad (u_{yy})_{i,j} = \frac{1}{k^2}(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}).$$

Solution of Laplace's equation We apply the Laplace's equation at the nodal point (i, j). Inserting the above approximations in the Laplace's equation, we obtain

$$(u_{xx})_{i,j} + (u_{yy})_{i,j} = \frac{1}{h^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + \frac{1}{k^2}(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) = 0 \tag{5.22}$$

or $$(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + p^2(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) = 0, \text{ where } p = h/k. \tag{5.23}$$

If $h = k$, that is, $p = 1$ (called uniform mesh spacing), we obtain the difference approximation as

$$u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} = 0 \tag{5.24}$$

This approximation is called the *standard five point formula.* We can write this formula as

$$u_{i,j} = \frac{1}{4}(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}). \tag{5.25}$$

We observe that $u_{i,j}$ is obtained as the mean of the values at the four neighbouring points in the x and y directions.

The nodal points that are used in computations are given in Fig.5.4.

Remark 6 The nodes in the mesh are numbered in an orderly way. We number them from left to right and from top to bottom or from bottom to top. A typical numbering is given in Figs.5.5a, 5.5b.

Example 5.8 *Solve $u_{xx} + u_{yy} = 0$ numerically for the following mesh with uniform spacing and with boundary conditions as shown below in the figure 5.7.*

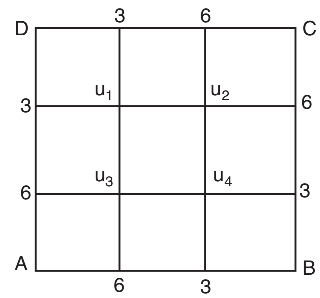

Fig. 5.7. Example 5.8.

Solution We note that the partial differential equation and the boundary conditions are symmetric about the diagonals *AC* and *BD.* Hence, $u_1 = u_4$ and $u_2 = u_3$. Therefore, we need to solve for two unknowns u_1 and u_2. We use the standard five point formula

$$u_{i+1,\, j} + u_{i-1,\, j} + u_{i,\, j+1} + u_{i,\, j-1} - 4u_{i,\, j} = 0.$$

We obtain the following difference equations.

At 1: $u_2 + 3 + 3 + u_3 - 4u_1 = 0,$

or $\quad -4u_1 + 2u_2 = -6,\quad$ or $\quad -2u_1 + u_2 = -3.$

At 2: $6 + 6 + u_1 + u_4 - 4u_2 = 0,\quad$ or $\quad 2u_1 - 4u_2 = -12.$

Adding the two equations, we get $-3u_2 = -15$, or $u_2 = 5$.

From the first equation, we get $\quad 2u_1 = u_2 + 3 = 5 + 3 = 8$, or $u_1 = 4$.

Example 5.9 *Solve $u_{xx} + u_{yy} = 0$ numerically for the following mesh with uniform spacing and with boundary conditions as shown below in the figure 5.8.*

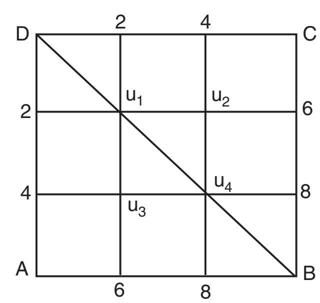

Fig. 5.8. Example 5.9.

Solution We note that the partial differential equation and the boundary conditions are symmetric about the diagonal *BD.* Hence, $u_2 = u_3$ and we need to determine u_1, u_2 and u_4. We use the standard five point formula

$$u_{i+1,\, j} + u_{i-1,\, j} + u_{i,\, j+1} + u_{i,\, j-1} - 4u_{i,\, j} = 0.$$

We obtain the following difference equations.

At1: $\quad u_2 + 2 + 2 + u_3 - 4u_1 = 0,\quad$ or $\quad -4u_1 + 2u_2 = -4,\quad$ or $\quad -2u_1 + u_2 = -2.$

At 2 $\quad 6 + 4 + u_1 + u_4 - 4u_2 = 0,\quad$ or $\quad u_1 - 4u_2 + u_4 = -10.$

At 4: $\quad 8 + u_2 + u_3 + 8 - 4u_4 = 0,\quad$ or $\quad 2u_2 - 4u_4 = -16,\quad$ or $\quad u_2 - 2u_4 = -8.$

We solve the system of equations using the Gauss elimination method. We use the augmented matrix **[A|d].**

$$\left[\begin{array}{rrr|r} -2 & 1 & 0 & -2 \\ 1 & -4 & 1 & -10 \\ 0 & 1 & -2 & -8 \end{array}\right];\ \frac{R_1}{-2},\ \left[\begin{array}{rrr|r} 1 & -1/2 & 0 & 1 \\ 1 & -4 & 1 & -10 \\ 0 & 1 & -2 & -8 \end{array}\right];\ R_2 - R_1,\ \left[\begin{array}{rrr|r} 1 & -1/2 & 0 & 1 \\ 0 & -7/2 & 1 & -11 \\ 0 & 1 & -2 & -8 \end{array}\right];$$

$$\frac{R_2}{-(7/2)},\ \left[\begin{array}{rrr|r} 1 & -1/2 & 0 & 1 \\ 0 & 1 & -2/7 & 22/7 \\ 0 & 1 & -2 & -8 \end{array}\right];\ R_3 - R_2,\ \left[\begin{array}{rrr|r} 1 & -1/2 & 0 & 1 \\ 0 & 1 & -2/7 & 22/7 \\ 0 & 0 & -12/7 & -78/7 \end{array}\right].$$

Solving the last equation, we get $\qquad u_4 = \dfrac{78}{12} = 6.5.$

Substituting in the second equation, we get $\qquad u_2 = \dfrac{22}{7} + \dfrac{13}{7} = \dfrac{35}{7} = 5.$

Substituting in the first equation, we get $\qquad u_1 = 1 + \dfrac{5}{2} = 3.5.$

Example 5.10 *Solve $u_{xx} + u_{yy} = 0$ numerically for the following mesh with uniform spacing and with boundary conditions as shown below in the figure 5.9.*

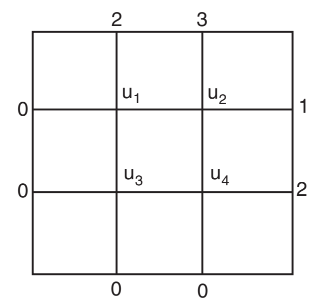

Fig. 5.9. Example 5.10.

Solution We note that the boundary conditions have no symmetry. Therefore, we need to find the values of the four unknowns u_1, u_2, u_3 and u_4. We use the standard five point formula

$$u_{i+1,\,j} + u_{i-1,\,j} + u_{i,\,j+1} + u_{i,\,j-1} - 4u_{i,\,j} = 0.$$

We obtain the following difference equations.

At1: $\quad u_2 + 2 + 0 + u_3 - 4u_1 = 0, \qquad$ or $\qquad -4u_1 + u_2 + u_3 = -2.$

At 2 $\quad 1 + 3 + u_1 + u_4 - 4u_2 = 0, \qquad$ or $\qquad u_1 - 4u_2 + u_4 = -4.$

At 3: $\quad u_4 + u_1 + 0 + 0 - 4u_3 = 0, \qquad$ or $\qquad u_1 - 4u_3 + u_4 = 0.$

At 4: $\quad 2 + u_2 + u_3 + 0 - 4u_4 = 0, \qquad$ or $\qquad u_2 + u_3 - 4u_4 = -2.$

We solve the system of equations using the Gauss elimination method. We use the augmented matrix **[A|d].**

$$\left[\begin{array}{rrrr|r} -4 & 1 & 1 & 0 & -2 \\ 1 & -4 & 0 & 1 & -4 \\ 1 & 0 & -4 & 1 & 0 \\ 0 & 1 & 1 & -4 & -2 \end{array}\right]; \frac{R_1}{-4}, \left[\begin{array}{rrrr|r} 1 & -1/4 & -1/4 & 0 & 1/2 \\ 1 & -4 & 0 & 1 & -4 \\ 1 & 0 & -4 & 1 & 0 \\ 0 & 1 & 1 & -4 & -2 \end{array}\right]; \; R_2 - R_1,\; R_3 - R_1,$$

$$\left[\begin{array}{rrrr|r} 1 & -1/4 & -1/4 & 0 & 1/2 \\ 0 & -15/4 & 1/4 & 1 & -9/2 \\ 0 & 1/4 & -15/4 & 1 & -1/2 \\ 0 & 1 & 1 & -4 & -2 \end{array}\right]; \frac{R_2}{\left(\dfrac{-15}{4}\right)}; \left[\begin{array}{rrrr|r} 1 & -1/4 & -1/4 & 0 & 1/2 \\ 0 & 1 & -1/15 & -4/15 & 18/15 \\ 0 & 1/4 & -15/4 & 1 & -1/2 \\ 0 & 1 & 1 & -4 & -2 \end{array}\right] \begin{array}{l} R_3 - \dfrac{1}{4} R_2, \\ R_4 - R_2, \end{array}$$

$$\left[\begin{array}{rrrr|r} 1 & -1/4 & -1/4 & 0 & 1/2 \\ 0 & 1 & -1/15 & -4/15 & 18/15 \\ 0 & 0 & -56/15 & 16/15 & -4/5 \\ 0 & 0 & 16/15 & -56/15 & -48/15 \end{array}\right] \frac{R_3}{(-56/15)}, \left[\begin{array}{rrrr|r} 1 & -1/4 & -1/4 & 0 & 1/2 \\ 0 & 1 & -1/15 & -4/15 & 18/15 \\ 0 & 0 & 1 & -16/56 & 12/56 \\ 0 & 0 & 16/15 & -56/15 & -48/15 \end{array}\right];$$

$$R_4 - \frac{16}{15}\, R_3, \left[\begin{array}{cccc|c} 1 & -1/4 & -1/4 & 0 & 1/2 \\ 0 & 1 & -1/15 & -4/15 & 18/15 \\ 0 & 0 & 1 & -16/56 & 12/56 \\ 0 & 0 & 0 & -2880/840 & -2880/840 \end{array}\right].$$

Last equation gives $u_4 = 1$.

Substituting in the third equation, we get $u_3 = \frac{12}{56} + \frac{16}{56} = \frac{28}{56} = 0.5$.

Substituting in the second equation, we get $u_2 = \frac{18}{15} + \frac{1}{30} + \frac{4}{15} = \frac{45}{30} = 1.5$.

Substituting in the first equation, we get $u_1 = \frac{1}{2} + \frac{3}{8} + \frac{1}{8} = 1.$

Example 5.11 *Solve $u_{xx} + u_{yy} = 0$ numerically under the boundary conditions*

$$u(x, 0) = 2x,\ u(0, y) = -y,$$

$$u(x, 1) = 2x - 1,\ u(1, y) = 2 - y$$

with square mesh of width $h = 1/3$.

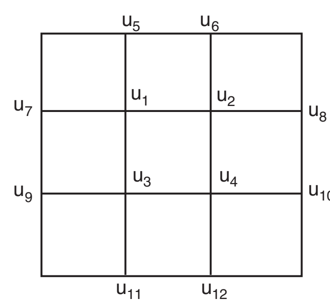

Fig. 5.10. Example 5.11.

Solution The mesh is given in Fig.5.10. We need to find the values of the four unknowns u_1, u_2, u_3 and u_4. We use the standard five point formula

$$u_{i+1, j} + u_{i-1, j} + u_{i, j+1} + u_{i, j-1} - 4u_{i, j} = 0.$$

Using the boundary conditions, we get the boundary values as

$$u_5 = u\left(\frac{1}{3}, 1\right) = \frac{2}{3} - 1 = -\frac{1}{3},\ u_6 = u\left(\frac{2}{3}, 1\right) = \frac{4}{3} - 1 = \frac{1}{3},\ u_7 = u\left(0, \frac{2}{3}\right) = -\frac{2}{3}$$

$$u_8 = u\left(1, \frac{2}{3}\right) = 2 - \frac{2}{3} = \frac{4}{3},\ u_9 = u\left(0, \frac{1}{3}\right) = -\frac{1}{3},\ u_{10} = u\left(1, \frac{1}{3}\right) = 2 - \frac{1}{3} = \frac{5}{3},$$

$$u_{11} = u\left(\frac{1}{3}, 0\right) = \frac{2}{3},\ u_{12} = u\left(\frac{2}{3}, 0\right) = \frac{4}{3}.$$

We obtain the following difference equations.

At1: $u_2 + u_5 + u_7 + u_3 - 4u_1 = 0$, or $-4u_1 + u_2 + u_3 = 1$.

At 2: $u_8 + u_6 + u_1 + u_4 - 4u_2 = 0$, or $u_1 - 4u_2 + u_4 = -5/3$.

At 3: $u_4 + u_1 + u_9 + u_{11} - 4u_3 = 0$, or $u_1 - 4u_3 + u_4 = -1/3$.

At 4: $u_{10} + u_2 + u_3 + u_{12} - 4u_4 = 0$, or $u_2 + u_3 - 4u_4 = -3$.

We solve the system of equations using the Gauss elimination method. We use the augmented matrix **[A|d]**.

$$\left[\begin{array}{cccc|c} -4 & 1 & 1 & 0 & 1 \\ 1 & -4 & 0 & 1 & -5/3 \\ 1 & 0 & -4 & 1 & -1/3 \\ 0 & 1 & 1 & -4 & -3 \end{array}\right];\ \frac{R_1}{-4},\ \left[\begin{array}{cccc|c} 1 & -0.25 & -0.25 & 0 & -0.25 \\ 1 & -4 & 0 & 1 & -5/3 \\ 1 & 0 & -4 & 1 & -1/3 \\ 0 & 1 & 1 & -4 & -3 \end{array}\right];\ R_2 - R_1,\ R_3 - R_1,$$

$$\left[\begin{array}{cccc|c} 1 & -0.25 & -0.25 & 0 & -0.25 \\ 0 & -3.75 & 0.25 & 1 & -1.41667 \\ 0 & 0.25 & -3.75 & 1 & -0.08333 \\ 0 & 1 & 1 & -4 & -3 \end{array}\right];\ \frac{R_2}{-3.75}$$

$$\left[\begin{array}{cccc|c} 1 & -0.25 & -0.25 & 0 & -0.25 \\ 0 & 1 & -0.06667 & -0.26667 & 0.37778 \\ 0 & 0.25 & -3.75 & 1 & -0.08333 \\ 0 & 1 & 1 & -4 & -3 \end{array}\right];$$

$$\begin{array}{r} R_3 - 0.25\,R_2, \\ R_4 - R_2, \end{array}\ \left[\begin{array}{cccc|c} 1 & -0.25 & -0.25 & 0 & -0.25 \\ 0 & 1 & -0.06667 & -0.26667 & 0.37778 \\ 0 & 0 & -3.73333 & 1.06667 & -0.17778 \\ 0 & 0 & 1.06667 & -3.73333 & -3.377778 \end{array}\right];\ \frac{R_3}{-3.73333},$$

$$\left[\begin{array}{cccc|c} 1 & -0.25 & -0.25 & 0 & -0.25 \\ 0 & 1 & -0.06667 & -0.26667 & 0.37778 \\ 0 & 0 & 1 & -0.28572 & -0.04762 \\ 0 & 0 & 1.06667 & -3.73333 & -3.37778 \end{array}\right];\quad R_4 - 1.06667\,R_3,$$

$$\left[\begin{array}{cccc|c} 1 & -0.25 & -0.25 & 0 & -0.25 \\ 0 & 1 & -0.06667 & -0.26667 & 0.37778 \\ 0 & 0 & 1 & -0.28572 & 0.04762 \\ 0 & 0 & 0 & -3.42856 & -3.42857 \end{array}\right].$$

Last equation gives $u_4 = 1$.

Substituting in the third equation, we get $u_3 = 0.04762 + 0.28572 = 0.33334$.

Substituting in the second equation, we get

$$u_2 = 0.37778 + 0.06667\ (0.33334) + 0.26667 = 0.66667.$$

Substituting in the first equation, we get $u_1 = -0.25 + 0.25(0.66667 + 0.33334) = 0$.

Example 5.12 *Solve the boundary value problem for the Poisson equation*

$$u_{xx} + u_{yy} = x^2 - 1,\ |\ x\ | \le 1,\ |\ y\ | \le 1,$$

$$u = 0 \textit{ on the boundary of the square}$$

using the five point formula with square mesh of width $h = 1/2$.

Solution The mesh is given in Fig.5.11. The partial differential equation and the boundary conditions are symmetric about x-and y-axis. We need to find the values of the four unknowns u_1, u_2, u_3 and u_4. We use the standard five point formula

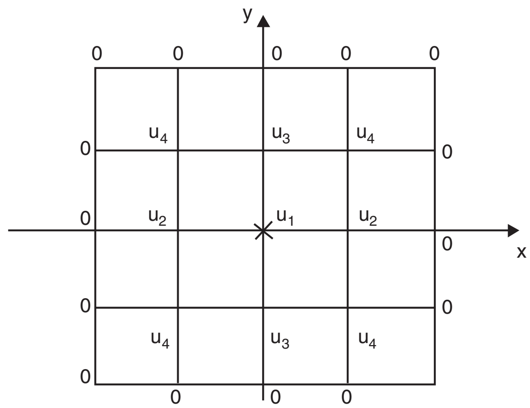

Fig. 5.11. Example 5.12.

$$u_{i+1, j} + u_{i-1, j} + u_{i, j+1} + u_{i, j-1} - 4u_{i, j} = h^2 G_{i, j} = 0.25(x_i^2 - 1).$$

We obtain the following difference equations.

At 1(0, 0): $\quad u_2 + u_3 + u_2 + u_3 - 4u_1 = -0.25,$

or $\quad -2u_1 + u_2 + u_3 = -0.125.$

At 2(0.5, 0): $\quad 0 + u_4 + u_1 + u_4 - 4u_2 = 0.25(0.25 - 1) = -0.1875,$

or $\quad u_1 - 4u_2 + 2u_4 = -0.1875.$

At 3(0, 0.5): $\quad u_4 + 0 + u_4 + u_1 - 4u_3 = 0.25(0 - 1) = -0.25,$

or $\quad u_1 - 4u_3 + 2u_4 = -0.25.$

At 4(0.5, 0.5): $\quad 0 + 0 + u_3 + u_2 - 4u_4 = 0.25(0.25 - 1) = -0.1875,$

or $\quad u_2 + u_3 - 4u_4 = -0.1875.$

We solve the system of equations using the Gauss elimination method. We use the augmented matrix **[A|d].**

$$\left[\begin{array}{rrrr|r} -2 & 1 & 1 & 0 & -0.125 \\ 1 & -4 & 0 & 2 & -0.1875 \\ 1 & 0 & -4 & 2 & -0.25 \\ 0 & 1 & 1 & -4 & -0.1875 \end{array}\right]; \frac{R_1}{-2}, \left[\begin{array}{rrrr|r} 1 & -0.5 & -0.5 & 0 & 0.0625 \\ 1 & -4 & 0 & 2 & -0.1875 \\ 1 & 0 & -4 & 2 & -0.25 \\ 0 & 1 & 1 & -4 & -0.1875 \end{array}\right]; R_2 - R_1, R_3 - R_1,$$

$$\left[\begin{array}{rrrr|r} 1 & -0.5 & -0.5 & 0 & 0.0625 \\ 0 & -3.5 & 0.5 & 2 & -0.25 \\ 0 & 0.5 & -3.5 & 2 & -0.3125 \\ 0 & 1 & 1 & -4 & -0.1875 \end{array}\right]; \frac{R_2}{-3.5}, \left[\begin{array}{rrrr|r} 1 & -0.5 & -0.5 & 0 & 0.0625 \\ 0 & 1 & -0.14286 & -0.57143 & 0.07143 \\ 0 & 0.5 & -3.5 & 2 & -0.3125 \\ 0 & 1 & 1 & -4 & -0.1875 \end{array}\right];$$

$$\begin{array}{l} R_3 - 0.5\,R_2, \\ R_4 - R_2, \end{array} \left[\begin{array}{cccc|c} 1 & -0.5 & -0.5 & 0 & 0.0625 \\ 0 & 1 & -0.14286 & -0.57143 & 0.07143 \\ 0 & 0 & -3.42857 & 2.28572 & -0.34822 \\ 0 & 0 & 1.14286 & -3.42857 & -0.25893 \end{array}\right]; \quad \frac{R_3}{-3.42857},$$

$$\left[\begin{array}{cccc|c} 1 & -0.5 & -0.5 & 0 & 0.0625 \\ 0 & 1 & -0.14286 & -0.57143 & 0.07143 \\ 0 & 0 & 1 & -0.66667 & 0.10156 \\ 0 & 0 & 1.14286 & -3.42857 & -0.25893 \end{array}\right]; \quad R_4 - 1.14286\,R_3,$$

$$\left[\begin{array}{cccc|c} 1 & -0.5 & -0.5 & 0 & 0.0625 \\ 0 & 1 & -0.14286 & -0.57143 & 0.07143 \\ 0 & 0 & 1 & -0.66667 & 0.10156 \\ 0 & 0 & 0 & -2.66667 & -0.37500 \end{array}\right].$$

Last equation gives $u_4 = \dfrac{0.37500}{2.66667} = 0.14062.$

Substituting in the third equation, we get $u_3 = 0.10156 + 0.66667(0.14062) = 0.19531.$

Substituting in the second equation, we get

$$u_2 = 0.07143 + 0.14286(0.19531) + 0.57143(0.14062) = 0.17969.$$

Substituting in the first equation, we get $u_1 = 0.5(0.17969 + 0.19531) + 0.0625 = 0.25.$

Iterative methods We mentioned earlier that when the order of the system of equations is large, which is the case in most practical problems, we use iterative methods. In fact, in many practical applications, we encounter thousands of equations. There are many powerful iterative methods available in the computer software, which are variants of successive over relaxation (SOR) method, conjugate gradient method etc. However, we shall discuss here, the implementation of the Gauss-Seidel method for the solution of the system of equations obtained in the application of the finite difference methods. Let us recall the properties of the Gauss-Seidel method.

(*a*) A sufficient condition for convergence is that the coefficient matrix **A**, of the system of equations is diagonally dominant.

(*b*) The method requires an initial approximation to the solution vector **u**. If no suitable approximation is available, then **u = 0** can be taken as the initial approximation.

(*c*) Using the initial approximations, we update the value of the first unknown u_1. Using this updated value of u_1 and the initial approximations to the remaining variables, we update the value of u_2. We continue until all the values are updated. We repeat the procedure until the required accuracy is obtained.

Liebmann iteration We use the above procedure to compute the solution of the difference equations for the Laplace's equation or the Poisson equation.

The initial approximations are obtained by judiciously using the standard five point formula (5.25)

5. R is a square of side 3 units. Boundary conditions are $u(0, y) = 0$, $u(3, y) = 3 + y$, $u(x, 0) = x$, $u(x, 3) = 2x$. Assume step length as $h = 1$.

6. R is a square of side 1 unit. $u(x, y) = x - y$ on the boundary. Assume $h = 1/3$.

Find the solution of the Poisson's equation $u_{xx} + u_{yy} = G(x, y)$ in the region R, subject to the given boundary conditions.

7. $R : 0 \le x \le 1, 0 \le y \le 1$. $G(x, y) = 4$. $u(x, y) = x^2 + y^2$ on the boundary and $h = 1/3$.

8. $R : 0 \le x \le 1, 0 \le y \le 1$. $G(x, y) = 3x + 2y$. $u(x, y) = x - y$ on the boundary and $h = 1/3$.

9. $R : 0 \le x \le 3, 0 \le y \le 3$. $G(x, y) = x^2 + y^2$. $u(x, y) = 0$ on the boundary and $h = 1$.

10. In Problems 2, 3, 4, 8, 9, solve the system of equations using the Liebmann iteration. In Problem 2, take the value at the top left hand point as – 2. In Problem 3, take the value at the top left hand point as 300. In Problem 4, take the value at the top left hand point as 0.Perform four iterations in each case.

5.5 FINITE DIFFERENCE METHOD FOR HEAT CONDUCTION EQUATION

In section 5.3, we have defined the linear second order partial differential equation

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu + G = 0$$

as a parabolic equation if $B^2 - AC = 0$. A parabolic equation holds in an open domain or in a semi-open domain. A parabolic equation together with the associated conditions is called an initial value problem or an initial-boundary value problem. The simplest example of a parabolic equation is the following problem.

Consider a thin homogeneous, insulated bar or a wire of length l. Let the bar be located on the x-axis on the interval $[0, l]$. Let the rod have a source of heat. For example, the rod may be heated at one end or at the middle point or has some source of heat. Let $u(x, t)$ denote the temperature in the rod at any instant of time t. The problem is to study the flow of heat in the rod. The partial differential equation governing the flow of heat in the rod is given by the parabolic equation

$$u_t = c^2 u_{xx},\ 0 \le x \le l,\ t > 0. \tag{5.35}$$

where c^2 is a constant and depends on the material properties of the rod. In order that the solution of the problem exists and is unique, we need to prescribe the following conditions.

(*i*) *Initial condition* At time $t = 0$, the temperature is prescribed, $u(x, 0) = f(x)$, $0 \le x \le l$.

(*ii*) *Boundary conditions* Since the bar is of length l, boundary conditions at $x = 0$ and at $x = l$ are to be prescribed. These conditions are of the following types:

(*a*) Temperatures at the ends of the bar is prescribed

$$u(0, t) = g(t),\ u(l, t) = h(t),\ t > 0. \tag{5.36}$$

(*b*) One end of the bar, say at $x = 0$, is insulated. This implies the condition that

$$\frac{\partial u}{\partial x} = 0, \text{ at } x = 0 \text{ for all time } t.$$

Note that the Bender-Schmidt method uses the value $\lambda = 1/2$. From the condition (5.45), we find that the higher order method (5.44), which uses the value $\lambda = 1/6$, is also stable.

Computational procedure

The initial condition $u(x, 0) = f(x)$ gives the solution at all the nodal points on the initial line (level 0). The boundary conditions $u(0, t) = g(t)$, $u(l, t) = h(t)$, $t > 0$ give the solutions at all the nodal points on the boundary lines $x = 0$ and $x = l$, (called boundary points), for all time levels. We choose a value for λ and h. This gives the value of the time step length k. Alternately, we may choose the values for h and k. The solutions at all nodal points, (called interior points), on level 1 are obtained using the explicit method. The computations are repeated for the required number of steps. If we perform m steps of computation, then we have computed the solutions up to time $t_m = mk$.

Let us illustrate the method through some problems.

Example 5.16 *Solve the heat conduction equation*

$$u_t = u_{xx},\ 0 \le x \le 1,\ \textit{with}\ u(x, 0) = \sin(\pi x),\ 0 \le x \le 1,\ u(0, t) = u(1, t) = 0$$

using the Schmidt method. Assume $h = 1/3$. *Compute with* (*i*) $\lambda = 1/2$ *for two time steps,* (*ii*) $\lambda = 1/4$ *for four time steps,* (*iii*) $\lambda = 1/6$ *for six time steps. If the exact solution is* $u(x, t) = \exp(-\pi^2 t) \sin(\pi x)$, *compare the solutions at time* $t = 1/9$.

Solution The Schmidt method is given by

$$u_{i,\, j+1} = \lambda u_{i-1,\, j} + (1 - 2\lambda) u_{i,\, j} + \lambda u_{i+1,\, j}$$

We are given $h = 1/3$. Hence, we have four nodes on each mesh line (see Fig.5.22). We have to find the solution at the two interior points.

The initial condition gives the values

$$u\left(\frac{1}{3}, 0\right) = u_{1,0} = \sin\left(\frac{\pi}{3}\right) = \frac{\sqrt{3}}{2},$$

$$u\left(\frac{2}{3}, 0\right) = u_{2,0} = \sin\left(\frac{2\pi}{3}\right) = \frac{\sqrt{3}}{2} = 0.866025.$$

The boundary conditions give the values $u_{0,\, j} = 0, u_{3,\, j} = 0$, for all j.

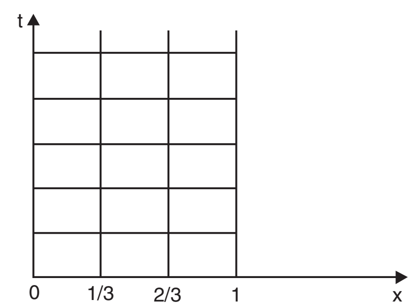

Fig. 5.22. Example. 5.16.

(*i*) We have $\lambda = 1/2$, $h = 1/3$, $k = \lambda h^2 = 1/18$. The computations are to be done for two time steps, that is, upto $t = 1/9$. For $\lambda = 1/2$, we get the method

$$u_{i,\, j+1} = \frac{1}{2}(u_{i-1,\, j} + u_{i+1,\, j}), \quad j = 0, 1\ ;\ i = 1, 2.$$

We have the following values.

For $j = 0$: $i = 1$: $\quad u_{1,\,1} = 0.5(u_{0,0} + u_{2,\,0}) = 0.5(0 + 0.866025) = 0.433013.$

$i = 2$: $\quad u_{2,\,1} = 0.5(u_{1,0} + u_{3,\,0}) = 0.5(0.866025 + 0) = 0.433013.$

For $j = 1$: $i = 1$: $u_{1,2} = 0.5(u_{0,1} + u_{2,1}) = 0.5(0 + 0.433013) = 0.216507.$

$i = 2$: $u_{2,2} = 0.5(u_{1,1} + u_{3,1}) = 0.5(0.433013 + 0) = 0.216507.$

After two steps $t = 2k = 1/9$. Hence,

$$u\left(\frac{1}{3}, \frac{1}{9}\right) = u\left(\frac{2}{3}, \frac{1}{9}\right) \approx 0.216507.$$

(*ii*) We have $\lambda = 1/4$, $h = 1/3$, $k = \lambda h^2 = 1/36$. The computations are to be done for four time steps, that is, upto $t = 1/9$. For $\lambda = 1/4$, we get the method

$$u_{i,\, j+1} = \frac{1}{4}\,(u_{i-1,\, j} + 2u_{i,\, j} + u_{i+1,\, j}), \quad j = 0, 1, 2, 3\ ;\ i = 1, 2.$$

We have the following values.

For $j = 0$: $i = 1$: $u_{1,1} = 0.25(u_{0,0} + 2u_{1,0} + u_{2,0}) = 0.25[0 + 3(0.866025)] = 0.649519.$

$i = 2$: $u_{2,1} = 0.25(u_{1,0} + 2u_{2,0} + u_{3,0}) = 0.25[3(0.866025) + 0] = 0.649519.$

For $j = 1$: $i = 1$: $u_{1,2} = 0.25(u_{0,1} + 2u_{1,1} + u_{2,1}) = 0.25[0 + 3(0.649519)] = 0.487139.$

$i = 2$: $u_{2,2} = 0.25(u_{1,1} + 2u_{2,1} + u_{3,1}) = 0.25[3(0.649519) + 0] = 0.487139.$

For $j = 2$: $i = 1$: $u_{1,3} = 0.25(u_{0,2} + 2u_{1,2} + u_{2,2}) = 0.25[0 + 3(0.487139)] = 0.365354.$

$i = 2$: $u_{2,3} = 0.25(u_{1,2} + 2u_{2,2} + u_{3,2}) = 0.25[3(0.487139) + 0] = 0.365354.$

For $j = 3$: $i = 1$: $u_{1,4} = 0.25(u_{0,3} + 2u_{1,3} + u_{2,3}) = 0.25[0 + 3(0.365354)] = 0.274016.$

$i = 2$: $u_{2,4} = 0.25(u_{1,3} + 2u_{2,3} + u_{3,3}) = 0.25[3(0.365354) + 0] = 0.274016.$

After four steps $t = 4k = 1/9$. Hence,

$$u\left(\frac{1}{3}, \frac{1}{9}\right) = u\left(\frac{2}{3}, \frac{1}{9}\right) \approx 0.274016,$$

(*iii*) We have $\lambda = 1/6$, $h = 1/3$, $k = \lambda h^2 = 1/54$. The computations are to be done for six time steps, that is, upto $t = 1/9$. For $\lambda = 1/6$, we get the method

$$u_{i,\, j+1} = \frac{1}{6}\,(u_{i-1,\, j} + 4u_{i,\, j} + u_{i+1,\, j}), \quad j = 0, 1, 2, 3, 4, 5\ ;\ i = 1, 2.$$

We have the following values.

For $j = 0$: $i = 1$: $u_{1,1} = \frac{1}{6}\,(u_{0,0} + 4u_{1,0} + u_{2,0}) = \frac{1}{6}\,[0 + 5(0.866025)] = 0.721688.$

$i = 2$: $u_{2,1} = \frac{1}{6}\,(u_{1,0} + 4u_{2,0} + u_{3,0}) = \frac{1}{6}\,[5(0.866025) + 0] = 0.721688.$

For $j = 1$: $i = 1$: $u_{1,2} = \frac{1}{6}\,(u_{0,1} + 4u_{1,1} + u_{2,1}) = \frac{1}{6}\,[0 + 5(0.721688)] = 0.601407.$

$i = 2$: $u_{2,2} = \frac{1}{6}\,(u_{1,1} + 4u_{2,1} + u_{3,1}) = \frac{1}{6}\,[5(0.721688) + 0] = 0.601407.$

For $j = 2$: $i = 1$: $u_{1,3} = \frac{1}{6}(u_{0,2} + 4u_{1,2} + u_{2,2}) = \frac{1}{6}[0 + 5(0.601407)] = 0.501173.$

$i = 2$: $u_{2,3} = \frac{1}{6}(u_{1,2} + 4u_{2,2} + u_{3,2}) = \frac{1}{6}[5(0.601407) + 0] = 0.501173.$

For $j = 3$: $i = 1$: $u_{1,4} = \frac{1}{6}(u_{0,3} + 4u_{1,3} + u_{2,3}) = \frac{1}{6}[0 + 5(0.501173)] = 0.417644.$

$i = 2$: $u_{2,4} = \frac{1}{6}(u_{1,3} + 4u_{2,3} + u_{3,3}) = \frac{1}{6}[5(0.501173) + 0] = 0.417644.$

For $j = 4$: $i = 1$: $u_{1,5} = \frac{1}{6}(u_{0,4} + 4u_{1,4} + u_{2,4}) = \frac{1}{6}[0 + 5(0.417644)] = 0.348037.$

$i = 2$: $u_{2,5} = \frac{1}{6}(u_{1,4} + 4u_{2,4} + u_{3,4}) = \frac{1}{6}[5(0.417644) + 0] = 0.348037.$

For $j = 5$: $i = 1$: $u_{1,6} = \frac{1}{6}(u_{0,5} + 4u_{1,5} + u_{2,5}) = \frac{1}{6}[0 + 5(0.348037)] = 0.290031.$

$i = 2$: $u_{2,6} = \frac{1}{6}(u_{1,5} + 4u_{2,5} + u_{3,5}) = \frac{1}{6}[5(0.348037) + 0] = 0.290031.$

After six steps $t = 6k = 1/9$. Hence,

$$u\left(\frac{1}{3}, \frac{1}{9}\right) = u\left(\frac{2}{3}, \frac{1}{9}\right) \approx 0.290031.$$

The magnitudes of errors at $x = 1/3$ and at $x = 2/3$ are same. The exact solution at $t = 1/9$ is

$$u\left(\frac{1}{3}, \frac{1}{9}\right) = u\left(\frac{2}{3}, \frac{1}{9}\right) = \exp\left(\frac{-\pi^2}{9}\right)\sin\left(\frac{\pi}{3}\right) \approx 0.289250.$$

The magnitudes of errors are the following:

$\lambda = 1/2$: $|\, 0.216507 - 0.289250 \,| = 0.072743.$

$\lambda = 1/4$: $|\, 0.274016 - 0.289250 \,| = 0.015234.$

$\lambda = 1/6$: $|\, 0.290031 - 0.289250 \,| = 0.000781.$

We note that the higher order method produced better results.

Example 5.17 *Solve* $u_{xx} = 32\, u_t$, $0 \le x \le 1$, *taking* $h = 0.5$ *and*

$$u(x, 0) = 0,\ 0 \le x \le 1, \quad u(0, t) = 0,\ u(1, t) = t,\ t > 0.$$

Use an explicit method with $\lambda = 1/2$. *Compute for four time steps.*

Solution The given partial differential equation is

$$u_t = \left(\frac{1}{32}\right) u_{xx} \text{ and } c^2 = \frac{1}{32}.$$

The step length is $h = 0.25$. We have five nodal points on each mesh line (see Fig.5.23). We are to find the solutions at three internal points.

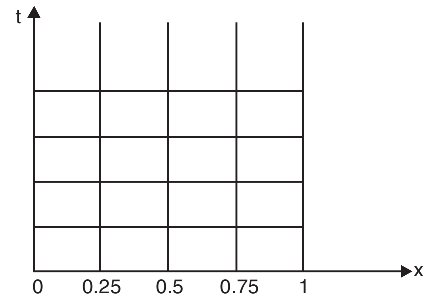

Fig. 5.23. Example 5.17.

The Schmidt method is given by

$$u_{i,\, j+1} = \lambda\, u_{i-1,\, j} + (1-2\lambda)u_{i,\, j} + \lambda u_{i+1,\, j}.$$

For $\lambda = 1/2$, the method becomes

$$u_{i,\, j+1} = 0.5\,(u_{i-1,\, j} + u_{i+1,\, j}),$$

$$j = 0, 1, 2, 3\ ;\ i = 1, 2, 3.$$

We have $$k = \frac{\lambda h^2}{c^2} = \frac{1}{2}\left(\frac{1}{16}\right)(32) = 1.$$

The initial condition gives the values $u_{0,\,0} = u_{1,0} = u_{2,0} = u_{3,0} = u_{4,0} = 0$.

The boundary conditions give the values $u_{0,\, j} = 0$, $u_{4,\, j} = t_j = jk = j$, for all j.

We obtain the following solutions.

For $j = 0$: $i = 1$: $u_{1,1} = 0.5(u_{0,0} + u_{2,0}) = 0.$

$i = 2$: $u_{2,1} = 0.5(u_{1,0} + u_{3,0}) = 0.$

$i = 3$: $u_{3,1} = 0.5(u_{2,0} + u_{4,0}) = 0.$

For $j = 1$: $i = 1$: $u_{1,2} = 0.5(u_{0,1} + u_{2,1}) = 0.5(0 + 0) = 0.$

$i = 2$: $u_{2,2} = 0.5(u_{1,1} + u_{3,1}) = 0.5(0 + 0) = 0.$

$i = 3$: $u_{3,2} = 0.5(u_{2,1} + u_{4,1}) = 0.5(0 + 1) = 0.5.$

For $j = 2$: $i = 1$: $u_{1,3} = 0.5(u_{0,2} + u_{2,2}) = 0.5(0 + 0) = 0.$

$i = 2$: $u_{2,3} = 0.5(u_{1,2} + u_{3,2}) = 0.5(0 + 0.5) = 0.25.$

$i = 3$: $u_{3,3} = 0.5(u_{2,2} + u_{4,2}) = 0.5(0 + 2) = 1.0.$

For $j = 3$: $i = 1$: $u_{1,4} = 0.5(u_{0,3} + u_{2,3}) = 0.5(0 + 0.25) = 0.125.$

$i = 2$: $u_{2,4} = 0.5(u_{1,3} + u_{3,3}) = 0.5(0 + 1.0) = 0.5.$

$i = 3$: $u_{3,4} = 0.5(u_{2,3} + u_{4,3}) = 0.5(0.25 + 3) = 1.625.$

The approximate solutions are $u(0.25, 4) \approx 0.125$, $u(0.5, 4) \approx 0.5$, $u(0.75, 4) \approx 1.625$.

Implicit methods

Explicit methods have the disadvantage that they have a stability condition on the mesh ratio parameter λ. We have seen that the Schmidt method is stable for $\lambda \le 0.5$. This condition severely restricts the values that can be used for the step lengths h and k. In most practical problems, where the computation is to be done up to large value of t, these methods are not useful because the time taken is too high. In such cases, we use the implicit methods. We shall discuss the most

Example 5.18 *Solve the equation $u_t = u_{xx}$ subject to the conditions*

$$u(x, 0) = \sin(\pi x),\ 0 \le x \le 1,\ u(0, t) = u(1, t) = 0$$

using the Crank-Nicolson method with, $h = 1/3$, $k = 1/36$. Do one time step.

(*A.U. Nov/Dec. 2006*)

Solution We have

$$c^2 = 1,\ h = \frac{1}{3},\ k = \frac{1}{36},\ \lambda = \frac{kc^2}{h^2} = \frac{1}{36}(9) = \frac{1}{4}. \qquad \text{(Fig.5.25).}$$

Crank-Nicolson method is given by

$$-\frac{\lambda}{2} u_{i-1, j+1} + (1+\lambda) u_{i, j+1} - \frac{\lambda}{2} u_{i+1, j+1} = \frac{\lambda}{2} u_{i-1, j} + (1-\lambda) u_{i, j} + \frac{\lambda}{2} u_{i+1, j}$$

For $\lambda = 1/4$, we have the method as

$$-\frac{1}{8} u_{i-1, j+1} + \frac{5}{4} u_{i, j+1} - \frac{1}{8} u_{i+1, j+1} = \frac{1}{8} u_{i-1, j} + \frac{3}{4} u_{i, j} + \frac{1}{8} u_{i+1, j}$$

or $$-u_{i-1, j+1} + 10u_{i, j+1} - u_{i+1, j+1} = u_{i-1, j} + 6u_{i, j} + u_{i+1, j}, \quad j = 0 ;\ i = 1, 2.$$

The initial condition gives the values

$$u_{0,0} = 0,\ u_{1,0} = \sin(\pi/3) = (\sqrt{3}/2) = u_{2,0},\ u_{3,0} = 0.$$

The boundary conditions give the values $u_{0, j} = 0 = u_{3, j}$ for all j,

We have the following equations.

For $j = 0$, $i = 1$: $\quad -u_{0,1} + 10\, u_{1,1} - u_{2,1} = u_{0,0} + 6u_{1,0} + u_{2,0}$

or $$10u_{1,1} - u_{2,1} = \frac{6\sqrt{3}}{2} + \frac{\sqrt{3}}{2} = \frac{7\sqrt{3}}{2} = 6.06218.$$

$i = 2$: $\quad -u_{1,1} + 10u_{2,1} - u_{3,1} = u_{1,0} + 6u_{2,0} + u_{3,0}$

or $$-u_{1,1} + 10u_{2,1} = u_{1,0} + 6u_{2,0} = \frac{\sqrt{3}}{2} + \frac{6\sqrt{3}}{2} = \frac{7\sqrt{3}}{2} = 6.06218.$$

Subtracting the two equations, we get $11u_{1,1} - 11u_{2,1} = 0$. Hence, $u_{1,1} = u_{2,1}$. The solution is given by

$$u_{1,1} = u_{2,1} = \frac{6.06218}{9} = 0.67358.$$

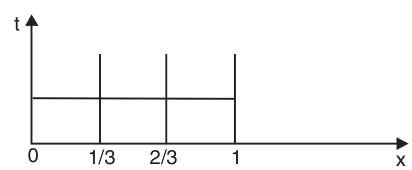

Fig. 5.25. Example 5.18.

Example 5.19 *Solve $u_{xx} = u_t$ in $0 < x < 2$, $t > 0$,*

$$u(0, t) = u(2, t) = 0,\ t > 0 \ \text{ and } u(x, 0) = \sin(\pi x/2),\ 0 \le x \le 2,$$

using $\Delta x = 0.5$, $\Delta t = 0.25$ for one time step by Crank-Nicolson implicit finite difference method.

(*A.U Apr/May 2003*)

Solution We have $c^2 = 1$, $\Delta x = 0.5$, $\Delta t = 0.25$, $\lambda = \dfrac{c^2 \Delta t}{\Delta x^2} = \dfrac{0.25}{0.25} = 1$.

Crank-Nicolson implicit finite difference method is given by

$$-\frac{\lambda}{2} u_{i-1, j+1} + (1+\lambda) u_{i, j+1} - \frac{\lambda}{2} u_{i+1, j+1} = \frac{\lambda}{2} u_{i-1, j} + (1-\lambda) u_{i, j} + \frac{\lambda}{2} u_{i+1, j}.$$

For $\lambda = 1$, we have the method as

$$-\frac{1}{2} u_{i-1, j+1} + 2u_{i, j+1} - \frac{1}{2} u_{i+1, j+1} = \frac{1}{2} u_{i-1, j} + \frac{1}{2} u_{i+1, j}$$

or $$-u_{i-1, j+1} + 4u_{i, j+1} - u_{i+1, j+1} = u_{i-1, j} + u_{i+i, j}, \quad j = 0\ ;\ i = 1, 2, 3,$$

The initial condition gives the values

$$u_{0,0} = 0,\ u_{1,0} = \sin(\pi/4) = (1/\sqrt{2}) = 0.70711,$$

$$u_{2,0} = \sin(\pi/2) = 1,\ u_{3,0} = \sin(3\pi/4) = (1/\sqrt{2}) = 0.70711.$$

The boundary conditions give the values $u_{0, j} = 0 = u_{4, j}$ for all j.

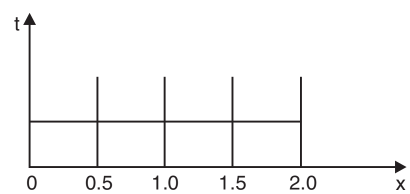

Fig. 5.26. Example 5.19.

We have the following equations.

For $j = 0, i = 1$: $\quad -u_{0,1} + 4u_{1,1} - u_{2,1} = u_{0,0} + u_{2,0}$ or $4u_{1,1} - u_{2,1} = 1$,

$i = 2$: $\quad -u_{1,1} + 4u_{2,1} - u_{3,1} = u_{1,0} + u_{3,0}$ or $-u_{1,1} + 4u_{2,1} - u_{3,1} = 1.41421$,

$i = 3$: $\quad -u_{2,1} + 4u_{3,1} - u_{4,1} = u_{2,0} + u_{4,0}$ or $-u_{2,1} + 4u_{3,1} = 1$.

Subtracting the first and third equations, we get $4u_{1,1} - 4u_{3,1} = 0$. Hence, $u_{1,1} = u_{3,1}$. We have the system of equations as

$$4u_{1,1} - u_{2,1} = 1, \text{ and } -2u_{1,1} + 4u_{2,1} = 1.41421.$$

Using determinants, the solution is obtained as

$$u_{1,1} = \frac{5.41421}{14} = 0.38673,\ u_{2,1} = \frac{7.65684}{14} = 0.54692.$$

Example 5.20 *Solve by Crank-Nicolson method the equation* $u_{xx} = u_t$ *subject to*

$$u(x, 0) = 0,\ u(0, t) = 0 \text{ and } u(1, t) = t,$$

for two time steps. (*A.U Nov/Dec. 2003, Nov/Dec. 2006*)

Solution Since the values of the step lengths h and k are not given, let us assume $h = 0.25$ and $\lambda = 1$. Hence, $k = \lambda h^2 = 0.0625$. (Fig. 5.27).

Crank-Nicolson implicit finite difference method is given by

$$-\frac{\lambda}{2}u_{i-1,j+1} + (1+\lambda)u_{i,j+1} - \frac{\lambda}{2}u_{i+1,\,j+1} = \frac{\lambda}{2}u_{i-1,j} + (1-\lambda)u_{i,j} + \frac{\lambda}{2}u_{i+1,j}.$$

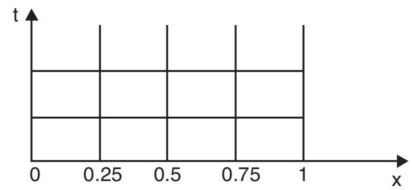

Fig. 5.27. Example 5.20.

For $\lambda = 1$, we have the method as

$$-\frac{1}{2}u_{i-1,j+1} + 2u_{i,j+1} - \frac{1}{2}u_{i+1,\,j+1} = \frac{1}{2}u_{i-1,j} + \frac{1}{2}u_{i+1,j}$$

or $$-u_{i-1,j+1} + 4u_{i,\,j+1} - u_{i+1,j+1} = u_{i-1,j} + u_{i+1,j},\quad j = 0\ ;\ i = 1, 2, 3..$$

The initial condition gives the values $u_{i,\,0} = 0$ for all i.

The boundary conditions give the values $u_{0,\,j} = 0$, for all j and $u_{4,\,j} = t_j = jk = 0.0625\,j$.

We have the following equations.

For $j = 0$, $\quad i = 1 : -u_{0,1} + 4u_{1,1} - u_{2,1} = u_{0,0} + u_{2,0}$ or $4u_{1,1} - u_{2,1} = 0$,

$i = 2 : -u_{1,1} + 4u_{2,1} - u_{3,1} = u_{1,0} + u_{3,0}$ or $-u_{1,1} + 4u_{2,1} - u_{3,1} = 0$,

$i = 3 : -u_{2,1} + 4u_{3,1} - u_{4,1} = u_{2,0} + u_{4,0}$ or $-u_{2,1} + 4u_{3,1} = 0.0625$.

The system of equations is given by

$$\begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix}\begin{bmatrix} u_{1,1} \\ u_{2,1} \\ u_{3,1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0.0625 \end{bmatrix}.$$

We solve this system by Gauss elimination.

$$\begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 0.0625 \end{bmatrix}, \text{ Perform } \frac{R_1}{4}, \text{ then } R_2 + R_1.\ \left[\begin{array}{ccc|c} 1 & -1/4 & 0 & 0 \\ 0 & 15/4 & -1 & 0 \\ 0 & -1 & 4 & 0.0625 \end{array}\right],$$

$$\text{Perform } \frac{R_2}{(15/4)}, \text{ then } R_3 + R_2.\ \left[\begin{array}{ccc|c} 1 & -1/4 & 0 & 0 \\ 0 & 1 & -4/15 & 0 \\ 0 & 0 & 56/15 & 0.0625 \end{array}\right],$$

The last equation gives $u_{3,1} = 0.0625\left(\frac{15}{56}\right) = 0.01674$.

The second equation gives $u_{2,1} = \left(\frac{4}{15}\right)u_{3,1} = \left(\frac{4}{15}\right)0.01674 = 0.00446$.

The first equation gives $u_{1,1} = \left(\frac{1}{4}\right)u_{2,1} = \left(\frac{1}{4}\right)0.00446 = 0.00112$.

For $j = 1$, $i = 1:$ $-u_{0,2} + 4u_{1,2} - u_{2,2} = u_{0,1} + u_{2,1} = 0 + 0.00446,$

or $4u_{1,2} - u_{2,2} = 0.00446.$

$i = 2:$ $-u_{1,2} + 4u_{2,2} - u_{3,2} = u_{1,1} + u_{3,1} = 0.00112 + 0.01674 = 0.01786.$

$i = 3:$ $-u_{2,2} + 4u_{3,2} - u_{4,2} = u_{2,1} + u_{4,1} = 0.00446 + 0,$

or $-u_{2,2} + 4u_{3,2} = 0.00446 + 0.125 = 0.12946.$

The system of equations is given by

$$\begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} u_{1,2} \\ u_{2,2} \\ u_{3,2} \end{bmatrix} = \begin{bmatrix} 0.00446 \\ 0.01786 \\ 0.12946 \end{bmatrix}.$$

We solve this system by Gauss elimination.

$$\left[\begin{array}{ccc|c} 4 & -1 & 0 & 0.00446 \\ -1 & 4 & -1 & 0.01786 \\ 0 & -1 & 4 & 0.12946 \end{array}\right]. \text{ Perform } \frac{R_1}{4}, \text{ then } R_2 + R_1. \left[\begin{array}{ccc|c} 1 & -1/4 & 0 & 0.001115 \\ 0 & 15/4 & -1 & 0.018975 \\ 0 & -1 & 4 & 0.12946 \end{array}\right].$$

$$\text{Perform } \frac{R_2}{(15/4)}, \text{ then } R_3 + R_2. \left[\begin{array}{ccc|c} 1 & -1/4 & 0 & 0.001115 \\ 0 & 1 & -4/15 & 0.00506 \\ 0 & 0 & 56/15 & 0.13452 \end{array}\right].$$

The last equation gives $u_{3,2} = \left(\frac{15}{56}\right) 0.13452 = 0.036032.$

The second equation gives $u_{2,2} = \left(\frac{4}{15}\right) u_{3,2} = \left(\frac{4}{15}\right) 0.036032 = 0.014669.$

The first equation gives $u_{1,2} = \left(\frac{1}{4}\right) u_{2,2} = \left(\frac{1}{4}\right) 0.014669 = 0.004782.$

REVIEW QUESTIONS

1. Write the one dimensional heat conduction equation and the associated conditions.

Solution The heat conduction equation is given by

$$u_t = c^2 u_{xx},\ 0 \le x \le l,\ t > 0.$$

The associated conditions are the following.

Initial condition At time $t = 0$, the temperature is prescribed, $u(x, 0) = f(x)$, $0 \le x \le l$.

Boundary conditions Since the bar is of length l, boundary conditions at $x = 0$ and at $x = l$ are to be prescribed.

$$u(0, t) = g(t),\ u(l, t) = h(t), \quad t > 0.$$

$$2u_{i,1} = 2(1 - r^2)u_{i,0} + r^2 [u_{i+1,0} + u_{i-1,0}]$$

or
$$u_{i,1} = (1 - r^2)u_{i,0} + \frac{r^2}{2} [u_{i+1,0} + u_{i-1,0}]. \quad (5.64)$$

For $r = 1$, the method simplifies to

$$u_{i,1} = \frac{1}{2} [u_{i+1,0} + u_{i-1,0}]. \quad (5.65)$$

Thus, the solutions at all nodal points on level 1 are obtained. For $t > k$, that is for $j \geq 1$, we use the method (5.56) or (5.59). The computations are repeated for the required number of steps. If we perform m steps of computation, then we have computed the solutions up to time $t_m = mk$.

Let us illustrate the method through some problems.

Example 5.21 *Solve the wave equation*

$u_{tt} = u_{xx}$, $0 \leq x \leq 1$, *subject to the conditions*

$u(x, 0) = \sin (\pi x)$, $u_t(x, 0) = 0$, $0 \leq x \leq 1$, $u(0, t) = u(1, t) = 0$, $t > 0$

using the explicit method with $h = 1/4$ *and (i)* $k = 1/8$, *(ii)* $k = 1/4$. *Compute for four time steps for (i), and two time steps for (ii). If the exact solution is* $u(x, t) = \cos (\pi t) \sin (\pi x)$, *compare the solutions at times* $t = 1/4$ *and* $t = 1/2$.

Solution The explicit method is given by

$$u_{i, j+1} = 2(1 - r^2)u_{i,j} + r^2 [u_{i+1,j} + u_{i-1, j}] - u_{i, j-1}.$$

We are given $c = 1$ and $h = 1/4$. Hence, we have five nodes on each time level (see Fig.5.30). We have to find the solution at three interior points.

The initial conditions give the values

(*a*) $u_{i,0} = \sin (i \pi/4)$, $i = 0, 1, 2, 3, 4$

$u_{0, 0} = 0$, $u_{1, 0} = \sin (\pi/4) = (1/\sqrt{2}) = 0.70711$, $u_{2,0} = \sin (\pi/2) = 1$,

$u_{3,0} = \sin (3\pi/4) = (1/\sqrt{2}) = 0.70711$, $u_{4,0} = \sin (\pi) = 0$.

(*b*) $u_t(x, 0) = 0$ gives $u_{i,-1} = u_{i, 1}$.

The boundary conditions give the values $u_{0, j} = 0$, $u_{4, j} = 0$, for all j.

(*i*) When $k = 1/8$, we get $r = \frac{k}{h} = \frac{1}{8}(4) = \frac{1}{2}$. The method becomes

$$u_{i, j+1} = 2\left(1 - \frac{1}{4}\right)u_{i,j} + \frac{1}{4}[u_{i+1,j} + u_{i-1,j}] - u_{i,j-1}$$

$$= 1.5u_{i, j} + 0.25[u_{i+1, j} + u_{i-1, j}] - u_{i, j-1},$$

$$j = 0, 1, 2, 3 \,;\; i = 1, 2, 3. \quad (5.66)$$

The computations are to be done for four time steps, that is, up to $t = 1/2$ or $j = 0, 1, 2, 3$.

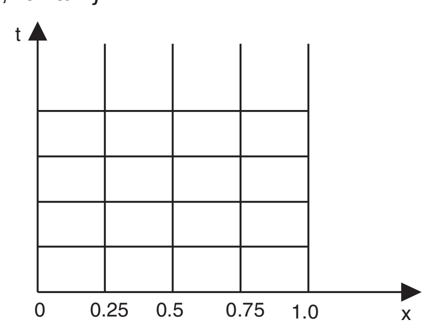

Fig. 5.30. Example. 5.21.

We have the following values.

For $j = 0$: Since $u_t(x, 0) = 0$ we obtain $u_{i,-1} = u_{i,1}$. The method simplifies to

$$u_{i,1} = 0.75u_{i,0} + 0.125[u_{i+1,0} + u_{i-1,0}].$$

$i = 1$: $$u_{1,1} = 0.75u_{1,0} + 0.125(u_{2,0} + u_{0,0})$$
$$= 0.75(0.70711) + 0.125(1 + 0) = 0.65533.$$

$i = 2$: $$u_{2,1} = 0.75u_{2,0} + 0.125(u_{3,0} + u_{1,0})$$
$$= 0.75 + 0.125(0.70711 + 0.70711) = 0.92678.$$

$i = 3$: $$u_{3,1} = 0.75u_{3,0} + 0.125(u_{4,0} + u_{2,0})$$
$$= 0.75(0.70711) + 0.125(0 + 1) = 0.65533.$$

For $j = 1$: We use the formula (5.66).

$i = 1$: $$u_{1,2} = 1.5u_{1,1} + 0.25[u_{2,1} + u_{0,1}] - u_{1,0}$$
$$= 1.5(0.65533) + 0.25(0.92678 + 0) - 0.70711 = 0.50758.$$

$i = 2$: $$u_{2,2} = 1.5\, u_{2,1} + 0.25[u_{3,1} + u_{1,1}] - u_{2,0}$$
$$= 1.5(0.92678) + 0.25(0.65533 + 0.65533) - 1.0 = 0.71784.$$

$i = 3$: $$u_{3,2} = 1.5u_{3,1} + 0.25[u_{4,1} + u_{2,1}] - u_{3,0}$$
$$= 1.5(0.65533) + 0.25(0 + 0.92678) - 0.70711 = 0.50758.$$

For $j = 2$:

$i = 1$: $$u_{1,3} = 1.5u_{1,2} + 0.25[u_{2,2} + u_{0,2}] - u_{1,1}$$
$$= 1.5(0.50758) + 0.25(0.71784 + 0) - 0.65533 = 0.28550.$$

$i = 2$: $$u_{2,3} = 1.5u_{2,2} + 0.25[u_{3,2} + u_{1,2}] - u_{2,1}$$
$$= 1.5(0.71784) + 0.25(0.50788 + 0.50788) - 0.92678 = 0.40377.$$

$i = 3$: $$u_{3,3} = 1.5u_{3,2} + 0.25[u_{4,2} + u_{2,2}] - u_{3,1}$$
$$= 1.5(0.50758) + 0.25(0 + 0.717835) - 0.65538 = 0.28550.$$

For $j = 3$:

$i = 1$: $$u_{1,4} = 1.5u_{1,3} + 0.25[u_{2,3} + u_{0,3}] - u_{1,2}$$
$$= 1.5(0.285499) + 0.25(0.403765 + 0) - 0.50758 = 0.02161.$$

$i = 2$: $$u_{2,4} = 1.5u_{2,3} + 0.25[u_{3,3} + u_{1,3}] - u_{2,2}$$
$$= 1.5(0.4037625) + 0.25(2)(0.285499) - 0.717835 = 0.03056.$$

$i = 3$: $$u_{3,4} = 1.5u_{3,3} + 0.25[u_{4,3} + u_{2,3}] - u_{3,2}$$
$$= 1.5(0.285499) + 0.25(0 + 0.40377) - 0.50758 = 0.02161.$$

(*ii*) When $k = 1/4$, $h = 1/4$, we get $r = \frac{k}{h} = \frac{1}{4}(4) = 1$. The computations are to be done for two time steps, that is, up to $t = 1/2$ or $j = 0, 1$. For $r = 1$, we get the method as

$$u_{i,j+1} = u_{i-1,j} + u_{i+1,j} - u_{i,j-1}, \quad j = 0, 1 \,;\; i = 1, 2, 3. \tag{5.67}$$

We have the following values.

For $j = 0$: $u_{i,-1} = u_{i,1}$, simplifies the method as

$$u_{i,1} = u_{i-1,0} + u_{i+1,0} - u_{i,1}, \text{ or } u_{i,1} = 0.5(u_{i-1,0} + u_{i+1,0}).$$

$i = 1$: $u_{1,1} = 0.5(u_{0,0} + u_{2,0}) = 0.5[0 + 1] = 0.5.$

$i = 2$: $u_{2,1} = 0.5(u_{1,0} + u_{3,0}) = 0.5(2)(0.70711) = 0.70711.$

$i = 3$: $u_{3,1} = 0.5(u_{2,0} + u_{4,0}) = 0.5(1 + 0) = 0.5.$

For $j = 1$: We use the formula (5.67).

$i = 1$: $u_{1,2} = u_{0,1} + u_{2,1} - u_{1,0} = 0 + 0.70711 - 0.70711 = 0.0$

$i = 2$: $u_{2,2} = u_{1,1} + u_{3,1} - u_{2,0} = 0.5 + 0.5 - 1.0 = 0.0.$

$i = 3$: $u_{3,2} = u_{2,1} + u_{4,1} - u_{3,0} = 0.70711 + 0 - 0.70711 = 0.0.$

The exact solution and the magnitudes of errors are as follows:

At $t = 0.25$: $u(0.25, 0.25) = u(0.75, 0.25) = 0.5$, $u(0.5, 0.25) = 0.70711$.

For $r = 1/2$: The magnitudes of errors are the following:

$| u(0.25, 0.25) - u_{1,2} | = | 0.50758 - 0.5 | = 0.00758,$

$| u(0.5, 0.25) - u_{2,2} | = | 0.717835 - 0.70711 | = 0.0107,$

$| u(0.75, 0.25) - u_{3,2} | = | 0.50758 - 0.5 | = 0.00758.$

For $r = 1$, we obtain the exact solution.

At $t = 0.5$: $u(0.25, 0.5) = u(0.75, 0.5) = u(0.5, 0.5) = 0.0$.

For $r = 1/2$: The magnitudes of errors are 0.02161, 0.03056, and 0.02161.

For $r = 1$, we obtain the exact solution.

Example 5.22 *Solve* $u_{tt} = 4u_{xx}$, *with boundary conditions* $u(0, t) = 0 = u(4, t)$, $t > 0$ *and the initial conditions* $u_t(x, 0) = 0$, $u(x, 0) = x(4 - x)$.

(*A.U., Nov/Dec 2006*)

Solution We have $c^2 = 4$. The values of the step lengths h and k are not prescribed. The number of time steps up to which the computations are to be performed is not prescribed. Therefore, let us assume that we use an explicit method with $h = 1$ and $k = 0.5$. Let the number of time steps up to which the computations are to be performed be 4. Then, we have

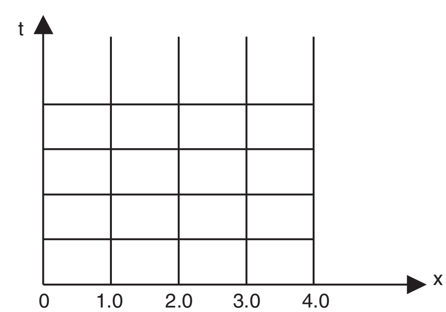

Fig. 5.31. Example 5.22.

$$r = \frac{ck}{h} = \frac{2(0.5)}{1} = 1.$$

The explicit formula is given by (see (5.59))

$$u_{i,j+1} = u_{i+1,j} + u_{i-1,j} - u_{i,j-1}, \quad j = 0, 1, 2, 3\ ;\ i = 1, 2, 3. \tag{5.68}$$

The boundary conditions give the values $u_{0,j} = 0$, $u_{4,j} = 0$, for all j (see Fig. 5.31).

The initial conditions give the following values.

$$u(x, 0) = x(4 - x), \text{ gives } u_{0,0} = 0,\ u_{1,0} = u(1, 0) = 3,$$

$$u_{2,0} = u(2, 0) = 4,\ u_{3,0} = u(3, 0) = 3,\ u_{4,0} = u(4, 0) = 0.$$

Central difference approximation to $u_t(x, 0) = 0$ gives $u_{i,-1} = u_{i,1}$.

We have the following results.

For $j = 0$: Since, $u_{i,-1} = u_{i,1}$, the formula simplifies to $u_{i,1} = 0.5(u_{i+1,0} + u_{i-1,0})$.

$i = 1$: $\quad u_{1,1} = 0.5(u_{2,0} + u_{0,0}) = 0.5(4 + 0) = 2,$

$i = 2$: $\quad u_{2,1} = 0.5(u_{3,0} + u_{1,0}) = 0.5(3 + 3) = 3,$

$i = 3$: $\quad u_{3,1} = 0.5(u_{4,0} + u_{2,0}) = 0.5(0 + 4) = 2.$

These are the solutions at the interior points on the time level $t = 0.5$.

For $j = 1$: We use the formula (5.68), to give $u_{i,2} = u_{i+1,1} + u_{i-1,1} - u_{i,0}$.

$i = 1$: $\quad u_{1,2} = u_{2,1} + u_{0,1} - u_{1,0} = 3 + 0 - 3 = 0,$

$i = 2$: $\quad u_{2,2} = u_{3,1} + u_{1,1} - u_{2,0} = 2 + 2 - 4 = 0,$

$i = 3$: $\quad u_{3,2} = u_{4,1} + u_{2,1} - u_{3,0} = 0 + 3 - 3 = 0.$

These are the solutions at the interior points on the time level $t = 1.0$.

For $j = 2$: We use the formula (5.68), to give $u_{i,3} = u_{i+1,2} + u_{i-1,2} - u_{i,1}$.

$i = 1$: $\quad u_{1,3} = u_{2,2} + u_{0,2} - u_{1,1} = 0 + 0 - 2 = -2,$

$i = 2$: $\quad u_{2,3} = u_{3,2} + u_{1,2} - u_{2,1} = 0 + 0 - 3 = -3,$

$i = 3$: $\quad u_{3,3} = u_{4,2} + u_{2,2} - u_{3,1} = 0 + 0 - 2 = -2.$

These are the solutions at the interior points on the time level $t = 1.5$.

For $j = 3$: We use the formula (5.68), to give $u_{i,4} = u_{i+1,3} + u_{i-1,3} - u_{i,2}$.

$i = 1$: $\quad u_{1,4} = u_{2,3} + u_{0,3} - u_{1,2} = -3 + 0 - 0 = -3,$

$i = 2$: $\quad u_{2,4} = u_{3,3} + u_{1,3} - u_{2,2} = -2 - 2 - 0 = -4,$

$i = 3$: $\quad u_{3,4} = u_{4,3} + u_{2,3} - u_{3,2} = 0 - 3 - 0 = -3.$

These are the solutions at the interior points on the required fourth time level $t = 2.0$.

Example 5.23 *Solve* $u_{xx} = u_{tt}$, $0 < x < 1$, $t > 0$, *given* $u(x, 0) = 0$, $u_t(x, 0) = 0$, $u(0, t) = 0$ *and* $u(1, t) = 100 \sin(\pi t)$. *Compute for four time steps with* $h = 0.25$. (*A.U. Nov/Dec. 2003*)

Solution We have $c = 1$ and $h = 0.25$, (see Fig. 5.30). The value of the step length k is not prescribed. Since the method is not specified, we use an explicit method.

We assume $k = 0.25$ so that $r = 1$. The method is given by

$$u_{i,j+1} = u_{i+1,j} + u_{i-1,j} - u_{i,j-1}, \quad j = 0, 1, 2, 3;\ i = 1, 2, 3.$$

The boundary conditions give the values

$u_{0,j} = 0$, for all j, and $u_{4,j} = 100 \sin(\pi jk) = 100 \sin(\pi j/4)$.

That is, $u_{4,0} = 0$, $u_{4,1} = 100 \sin(\pi/4) = (100/\sqrt{2}) = 50\sqrt{2}$,

$u_{4,2} = 100 \sin(\pi/2) = 100$,

$u_{4,3} = 100 \sin(3\pi/4) = (100/\sqrt{2}) = 50\sqrt{2}$, $u_{4,4} = 100 \sin(\pi) = 0$.

For $j = 0$: Since, $u_{i,-1} = u_{i,1}$, the formula simplifies to $u_{i,1} = 0.5(u_{i+1,0} + u_{i-1,0})$.

$i = 1$: $u_{1,1} = 0.5(u_{2,0} + u_{0,0}) = 0.5(0 + 0) = 0$,

$i = 2$: $u_{2,1} = 0.5(u_{3,0} + u_{1,0}) = 0.5(0 + 0) = 0$

$i = 3$: $u_{3,1} = 0.5(u_{4,0} + u_{2,0}) = 0.5(0 + 0) = 0$.

These are the solutions at the interior points on the time level $t = 0.25$.

For $j = 1$: We use the formula (5.68), to give $u_{i,2} = u_{i+1,1} + u_{i-1,1} - u_{i,0.}$

$i = 1$: $u_{1,2} = u_{2,1} + u_{0,1} - u_{1,0} = 0$,

$i = 2$: $u_{2,2} = u_{3,1} + u_{1,1} - u_{2,0} = 0$,

$i = 3$: $u_{3,2} = u_{4,1} + u_{2,1} - u_{3,0} = 50\sqrt{2} + 0 - 0 = 50\sqrt{2}$.

These are the solutions at the interior points on the time level $t = 0.5$.

For $j = 2$: We use the formula (5.68), to give $u_{i,3} = u_{i+1,2} + u_{i-1,2} - u_{i,1}$.

$i = 1$: $u_{1,3} = u_{2,2} + u_{0,2} - u_{1,1} = 0 + 0 + 0 = 0$,

$i = 2$: $u_{2,3} = u_{3,2} + u_{1,2} - u_{2,1} = 50\sqrt{2} + 0 - 0 = 50\sqrt{2}$,

$i = 3$: $u_{3,3} = u_{4,2} + u_{2,2} - u_{3,1} = 100 + 0 - 0 = 100$.

These are the solutions at the interior points on the time level $t = 0.75$.

For $j = 3$: We use the formula (5.68), to give $u_{i,4} = u_{i+1,3} + u_{i-1,3} - u_{i,2}$.

$i = 1$: $u_{1,4} = u_{2,3} + u_{0,3} - u_{1,2} = 50\sqrt{2} + 0 - 0 = 50\sqrt{2}$,

$i = 2$: $u_{2,4} = u_{3,3} + u_{1,3} - u_{2,2} = 100 + 0 - 0 = 100$,

$i = 3$: $u_{3,4} = u_{4,3} + u_{2,3} - u_{3,2} = 50\sqrt{2} + 50\sqrt{2} - 50\sqrt{2} = 50\sqrt{2}$.

These are the solutions at the interior points on the required fourth time level $t = 1.0$.

Indian Institute of Technolgy Indore

Semester: Spring

Course: Numerical Methods (MA-204)

Tutorial-IX

1. Describe the suitable smallest interval in which the following equations have roots:
   - $8x^3 - 12x^2 - 2x + 3 = 0$.
   - $\cos x - xe^x = 0$.
   - $\tan x + \tanh x = 0$.
   - $x^3 - x - 4 = 0$.
2. Find the root of $f(x) = x^3 - 3x + 1$ by Bisection method in the interval $[0, 1]$.
3. Use Bisection method to find a root of the equation $x = \cos x$ with absolute error less than 0.02. Also, solve by Newton method.
4. Find a zero of $f(x) = x^3 - 2x^2 + x - 3$ by Newton method with initial value $x_0 = 4$.
5. Find a zero of $f(x) = x^6 - x - 1$ by Secant method with initial values $x_0 = 1$ and $x_1 = 1.5$.
6. Find the positive solution of $f(x) = x - 2\sin x$ by the Secant method, starting from $x_0 = 2, x_1 = 1.9$.
7. Find the interval in which the smallest positive root of the following equations lies:

   (a) $\tan x + \tan hx = 0$

   (b) $x^3 - x - 4 = 0$.

   Determine the roots correct to two decimal places using the Bisection method.
8. Find the iterative methods based on the Newton-Raphson method for finding $\sqrt{N}, 1/N, N^{\frac{1}{3}}$, where N is a positive real number. Apply the methods to N = 18 to obtain the results correct to two decimal places.
9. The multiple root ξ of multiplicity two of the equation $f(x) = 0$ is to be determined. We consider the multipoint method

   $$x_{k+1} = x_k - \frac{f\left(x_k + 2\frac{f(x_k)}{f'(x_k)}\right)}{2f'(x_k)}.$$

   Show that the iteration method has third order rate of convergence. Hence, solve the equation

   $$9x^4 + 30x^3 + 34x^2 + 30x + 25 = 0 \quad \text{with} \quad x_0 = -1.4$$

   correct to three decimals.

10. Show that the following two sequences have convergence of the second order with the same limit $\sqrt{a}$

$$(i) x_{n+1} = \frac{x_n}{2}\left(1 + \frac{a}{x_n^2}\right), \qquad (ii) x_{k+1} = \frac{x_n}{2}\left(3 - \frac{x_n^2}{a}\right).$$

If x_n is a suitably close approximation to $\sqrt{a}$, show that the error in the first formula for x_{n+1} is about one-third of that in the second formula and deduce the following formula

$$x_{n+1} = \frac{1}{8} x_n \left(6 + \frac{3a}{x_n^2} - \frac{x_n^2}{a}\right),$$

gives a sequence with third-order convergence.

11. The equation $x^2 + ax + b = 0$ has two real roots α and β. Show that the iteration method

   (i) $x_{k+1} = -(ax_k + b)/x_k$ is convergent near x=α if $|\alpha| > |\beta|$.

   (ii) $x_{k+1} = -b/(x_k + a)$ is convergent near x=α if $|\alpha| < |\beta|$.

   (iii) $x_{k+1} = -(x_k^2 + b)/a$ is convergent near x=α if $2|\alpha| < |\alpha + \beta|$.

Indian Institute of Technolgy Indore

Semester: Spring

Course: Numerical Methods (MA-204)

Tutorial-X

1. Determine the order of convergence of the iterative method

$$x_{k+1} = \frac{x_0 f(x_k) - x_k f(x_0)}{f(x_k) - f(x_0)}$$

for finding a simple root of the equation $f(x) = 0$.

2. The system of equation

$$y\cos(xy) + 1 = 0$$

$$\sin(xy) + x - y = 0$$

has one solution close to $x = 1, y = 2$. Calculate this solution correct to 2 decimal places.

3. Obtain the complex roots of the equation

$$f(z) = z^3 + 1 = 0,$$

where z is complex variable, correct to eight decimal places. Use the initial approximation to the root as $(x_0, y_0) = (0.25, 0.25)$. Compare with the exact values of the roots $(1 \pm i\sqrt{3})/2$.

4. Compute an approximation to $y(1)$, $y'(1)$ and $y''(1)$ with Taylor's algorithm of order two and step length $h = 1$ when $y(x)$ is the solution to the initial value problem

$$y''' + 2y'' + y' - y = \cos x, 0 \leq x \leq 1, y(0) = 1, y'(0) = 1, y''(0) = 2.$$

5. Apply Taylor series method to order p to the problem $y' = y, y(0) = 1$ to show that

$$|y_n - y(x_n)| \leq \frac{h^p}{(p+1)!} x_n e^{x_n}.$$

6. Show that in Euler method, the bound of the truncation error when applied to the test equation $u' = \lambda u, u(a) = B, \lambda > 0$, can be written as

$$|u(t_j) - u(t_j, h)| \leq \frac{hM}{2\lambda}[exp\{\lambda(t_j - a)\} - 1]$$

where $M = \max|u''(t)|$. Generalise the result when applied to the problem $u' = f(t, u), u(a) = B$.

7. Consider the initial value problem $y' = x(y + x) - 2, y(0) = 2$. Use Euler's Method with step sizes $h = 0.3, h = 0.2$ and $h = 0.15$ to compute approximations to $y(0.6)$(5 decimals).

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Semester: Spring

Course: Numerical Methods (MA-204)

Tutorial-XI

1. Use the classical Runge-Kutta method of fourth order to find the numerical solution at $x = 0.8$ for
$$\frac{dy}{dx} = \sqrt{x+y}, \quad y(0.4) = 0.41.$$
Assume the step length $h = 0.2$.

2. Solve the initial value problem
$$u' = -2tu^2, u(0) = 1$$
with $h = 0.2$ on the interval $[0, 0.4]$. Use the second order implicit Runge-Kutta method.

3. Given the equation
$$y' = x + \sin y$$
with $y(0) = 1$, show that it is sufficient to use Euler's method with the step $h = 0.2$ to compute $y(0.2)$ with an error less than 0.05.

4. One method for the solution of the differential equation $y' = f(y)$ with $y(0) = y_0$ is the implicit mid-point method
$$y_{n+1} = y_n + hf\left(\frac{1}{2}(y_n + y_{n+1})\right).$$
Find the local error of this method.

5. Use the Taylor series method of order two, for step by step integration of the initial value problem
$$\begin{aligned} y' &= xz + 1, \quad y(0) = 0, \\ z' &= xy, \quad z(0) = 1, \end{aligned}$$
with $h = 0.1$ and $0 \leq x \leq 0.2$.

6. Solve the initial value problem
$$\begin{aligned} u' &= -3u + 2v, \quad u(0) = 0 \\ v' &= 3u - 4v, \quad v(0) = 0.5 \end{aligned}$$
with $h = 0.2$ on the interval $[0, 0.4]$, using the Runge-Kutta fourth order method.

7. Compute approximations to $y(0.4)$ and $y'(0.4)$, for the initial value problem
$$y'' + 4y = cost, y(0) = 1, y'(0) = 0$$
using Taylor series method of fourth order with step length $h = 0.2$. If exact solution is given by $y(t) = (2\cos 2t + \cos t)/3$, find the magnitudes of the errors.

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Tutorial-XII

1. Find an approximate value of $y(1.2)$ for the initial value problem

$$y' = x^2 + y^2, y(1) = 2$$

using the Adam-Moulton third order method

$$y_{i+1} = y_i + \frac{h}{12}[5f_{i+1} + 8f_i - f_{i-1}]$$

with $h = 0.1$.Calculate the starting value using third order Taylor series method with $h = 0.1$.

2. Obtain the constants a_1, b_1 and b_2 in the explicit multistep method

$$y_{i+1} = a_1 y_i + h[b_1 y_i' + b_2 y_{i-1}']$$

Determine the truncation error and the order of the method.

3. Obtain the approximate value of $y(0.3)$ for the initial value problem

$$y' = x^2 + y^2, y(0) = 1$$

using the method

$$\text{P=predictor} : y_{i+1}^{(p)} = y_i + hf_i$$

$$\text{C=corrector} : y_{i+1}^{(c)} = y_i + \frac{h}{2}[f_i + f(x_{i+1} + y_{i+1})]$$

with the step length $h = 0.1$.Perform two corrector iterations per step.

4. Solve the initial value problem

$$y' = x + y^2, y(0) = 1$$

in the interval [0,1] with the step length $h = 0.2$ using the multi-step method

$$y_{i+1} = y_i + \frac{h}{3}(23f_i - 16f_{i-1} + 5f_{i-2})$$

(Adams-Bashforth third order method). Compute the starting values using third order Taylor series method with the same step size h.

5. For the initial value problem

$$u' = t + u, \quad u(0) = 1$$

estimate $u(0.5)$ using the third order Adams-Moulton method.

6. Show that the Milne-Simpson method

$$y_{n+1} = y_{n-1} + \frac{h}{3}(y_{n+1}' + 4y_n' + y_{n-1}')$$

is not absolutely stable for any h.

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Course: Numerical Methods (MA-204)

Tutorial-XIII

1. Solve $u_{xx} = u_{tt}, 0 < x < 1, t > 0$, given $u(x, 0) = 0, u_t(x, 0) = 0, u(0, t) = 0$ and $u(1, t) = 100sin(\pi t)$. Compute for four time steps with $h = 0.25$.

2. Solve the wave equation $u_{tt} = u_{xx}, 0 \leq x \leq 1$, subject to the conditions

$$u(x, 0) = sin(\pi x),\ u_t(x, 0) = 0,\ 0 \leq x \leq 1,\ u(0, t) = u(1, t) = 0, t > 0$$

using the explicit method with $h = 1/4$ and (i) $k = 1/8$, (ii) $k = 1/4$. Compute for four time steps for (i), and two time steps for (ii). If the exact solution is $u(x, t) = cos(\pi t)sin(\pi x)$, compare the solutions at times $t = 1/4$ and $t = 1/2$.

3. Solve the boundary value problem

$$(1 + x^2)y'' + 4xy' + 2y = 2,\ y(0) = 0,\ y(1) = 1/2$$

by finite difference method. Use central difference approximations with $h = 1/3$.

4. Using the second order finite difference method, find $y(0.25),\ y(0.5),\ y(0.75)$ satisfying the differential equation $y'' - y' = x$ and subject to the conditions $y(0) = 0, y(1) = 2$.

5. Classify the following partial differential equations.

   - $u_{xx} + 4u_{yy} - u_x - 2u_y = 0$.
   - $u_{xx} - u_{yy} + 3u_x + 4u_y = 0$.
   - $u_{xx} + 4xu_{xy} + (1 - 4y^2)u_{yy} = 0$.
   - $u_{tt} + (5 + 2x^2)u_{xt} + (1 + x^2)(4 + x^2)u_{xx} = 0$.
   - $u_{xx} + 4u_{xy} + (x^2 + 4y^2)u_{yy} = x^2 + y^2$.

6. Solve the heat conduction equation $u_t = u_{xx}, 0 \leq x \leq 1$, with $u(x, 0) = sin(\pi x), 0 \leq x \leq 1,\ u(0, t) = u(1, t) = 0$ using the Schmidt method. Assume $h = 1/3$. Compute with (i) $\lambda = 1/2$ for two time steps, (ii) $\lambda = 1/4$ for four time steps, (iii) $\lambda = 1/6$ for six time steps. If the exact solution is $u(x, t) = exp(-\pi^2 t)sin(\pi x)$, compare the solutions at time $t = 1/9$.

7. Solve $u_{xx} = u_t$ in $0 < x < 2, t > 0$,

$$u(0, t) = u(2, t) = 0, t > 0,\ u(x, 0) = sin(\pi x/2), 0 \leq x \leq 2,$$

using $\Delta x = 0.5, \Delta t = 0.25$ for one time step by Crank-Nicolson implicit finite difference method.