

Lecture 06: Roots-Open Methods

Bangladesh University of Eng. & Tech. Slide 1 of 62 Industrial & Production Engineering

Bracketing Methods vs. Open Methods

- For the bracketing methods, the root is located within an interval prescribed by a lower and an upper bound.
- Repeated application of these methods always results in closer estimates of the true value of the root.
- Such methods are said to be **convergent** because they move closer to the truth as the computation progresses.
- In contrast, the open methods require only a single starting value or two starting values that do not necessarily bracket the root.
- As such, they sometimes **diverge** or move away from the true root as the computation progresses.
- However, when the open methods converge they usually do so much more quickly than the bracketing methods.

Bangladesh University of Eng. & Tech. Slide 2 of 62 Industrial & Production Engineering

Bracketing Methods vs. Open Methods

Bangladesh University of Eng. & Tech. Slide 3 of 62 Industrial & Production Engineering

Simple Fixed-point Iteration (FPI)

- Also known as **one-point iteration** or **successive substitution**.
- FPI derives an updating formula by rearranging the function as follows:

$$x = g(x)$$

$$x^2 - 2x + 3 = 0 \implies x = \frac{x^2 + 3}{2}$$

$$\sin x = 0 \implies x = \sin x + x$$

Bangladesh University of Eng. & Tech. Slide 4 of 62 Industrial & Production Engineering

Simple Fixed-point Iteration (FPI)

$$x_{i+1} = g(x_i)$$

$$\epsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| 100\%$$

Bangladesh University of Eng. & Tech. Slide 5 of 62 Industrial & Production Engineering

Example 1

Problem Statement. Use simple fixed-point iteration to locate the root of $f(x) = e^{-x} - x$.

$$x_{i+1} = e^{-x_i}$$

| i | x_i | ϵ_a (%) | ϵ_t (%) |
|----|----------|------------------|------------------|
| 0 | 0 | | 100.0 |
| 1 | 1.000000 | 100.0 | 76.3 |
| 2 | 0.367879 | 171.8 | 35.1 |
| 3 | 0.692201 | 46.9 | 22.1 |
| 4 | 0.500473 | 38.3 | 11.8 |
| 5 | 0.606244 | 17.4 | 6.89 |
| 6 | 0.545396 | 11.2 | 3.83 |
| 7 | 0.579612 | 5.90 | 2.20 |
| 8 | 0.560115 | 3.48 | 1.24 |
| 9 | 0.571143 | 1.93 | 0.705 |
| 10 | 0.564879 | 1.11 | 0.399 |

true value of the root: 0.56714329

Bangladesh University of Eng. & Tech. Slide 6 of 62 Industrial & Production Engineering

Convergence

- Notice that the true percent relative error for each iteration of the previous example is roughly proportional (by a factor of about 0.5 to 0.6) to the error from the previous iteration.
- This property, called **linear convergence**, is characteristic of fixed-point iteration.
- We must comment at this point about the “possibility” of convergence.
- The **two-curve method** (an alternative graphical approach) can be used to illustrate the convergence and divergence of fixed-point iteration.

Bangladesh University of Eng. & Tech. Slide 7 of 62 Industrial & Production Engineering

Two-curve Method

- It separates the equation into two component parts:

$$f_1(x) = f_2(x)$$

$$y_1 = f_1(x) \quad y_2 = f_2(x)$$
- These two equations can be plotted separately.
- The x values corresponding to the intersections of these functions represent the roots of $f(x) = 0$.

Bangladesh University of Eng. & Tech. Slide 8 of 62 Industrial & Production Engineering

Example 2

Problem Statement. Separate the equation $e^{-x} - x = 0$ into two parts and determine its root graphically.

$y_1 = x$ and $y_2 = e^{-x}$

| x | y ₁ | y ₂ |
|-----|----------------|----------------|
| 0.0 | 0.0 | 1.000 |
| 0.2 | 0.2 | 0.819 |
| 0.4 | 0.4 | 0.670 |
| 0.6 | 0.6 | 0.549 |
| 0.8 | 0.8 | 0.449 |
| 1.0 | 1.0 | 0.368 |

Bangladesh University of Eng. & Tech. Slide 9 of 62 Industrial & Production Engineering

Example 2

Bangladesh University of Eng. & Tech. Slide 10 of 62 Industrial & Production Engineering

Two-curve Method

$x = g(x)$

$$y_1 = x \quad y_2 = g(x)$$

Bangladesh University of Eng. & Tech. Slide 11 of 62 Industrial & Production Engineering

Two-curve Method

Bangladesh University of Eng. & Tech. Slide 12 of 62 Industrial & Production Engineering

Convergence of FPI

- For the first case (Fig. a), the initial guess of x_0 is used to determine the corresponding point on the y_2 curve [$x_0, g(x_0)$].
- The point (x_1, x_1) is located by moving left horizontally to the y_1 curve.
- These movements are equivalent to the first iteration in the fixed-point method:

$$x_1 = g(x_0)$$

Bangladesh University of Eng. & Tech. Slide 13 of 62 Industrial & Production Engineering

Convergence of FPI

- The next iteration consists of moving to $[x_1, g(x_1)]$ and then to (x_2, x_2) .
- This iteration is equivalent to the equation

$$x_2 = g(x_1)$$

- Notice that convergence seems to occur only when the absolute value of the slope of $y_2 = g(x)$ is less than the slope of $y_1 = x$, that is, when $|g'(x)| < 1$.

Bangladesh University of Eng. & Tech. Slide 14 of 62 Industrial & Production Engineering

Convergence of FPI: Theoretical Derivation

$$x_{i+1} = g(x_i)$$

$$x_r = g(x_r)$$

$$x_r - x_{i+1} = g(x_r) - g(x_i)$$

The *derivative mean-value theorem* (recall Sec. 4.1.1) states that if a function $g(x)$ and its first derivative are continuous over an interval $a \leq x \leq b$, then there exists at least one value of $x = \xi$ within the interval such that

$$g'(\xi) = \frac{g(b) - g(a)}{b - a}$$

Bangladesh University of Eng. & Tech. Slide 15 of 62 Industrial & Production Engineering

Convergence of FPI: Theoretical Derivation

If the true error for iteration i is defined as

$$E_{t,i} = x_r - x_i$$

$$E_{t,i+1} = g'(\xi)E_{t,i}$$

Bangladesh University of Eng. & Tech. Slide 16 of 62 Industrial & Production Engineering

Convergence of FPI: Theoretical Derivation

$$E_{t,i+1} = g'(\xi)E_{t,i}$$

- Consequently, if $|g'(x)| < 1$, the errors decrease with each iteration.
- For $|g'(x)| > 1$, the errors grow.
- Notice also that if the derivative is positive, the errors will be positive, and hence, the iterative solution will be monotonic (Fig. a and c).
- If the derivative is negative, the errors will oscillate (Fig. b and d).
- When the method converges, the error is roughly proportional to and less than the error of the previous step.
- For this reason, simple fixed point iteration is said to be **linearly convergent**.

Bangladesh University of Eng. & Tech. Slide 17 of 62 Industrial & Production Engineering

Algorithm for Fixed-Point Iteration

```

FUNCTION Fixpt(x0, es, imax, iter, ea)
  xr = x0
  iter = 0
  DO
    xrold = xr
    xr = g(xrold)
    iter = iter + 1
    IF xr ≠ 0 THEN
      ea = | (xr - xrold) / xr | * 100
    END IF
    IF ea < es OR iter ≥ imax EXIT
  END DO
  Fixpt = xr
END Fixpt
    
```

Bangladesh University of Eng. & Tech. Slide 18 of 62 Industrial & Production Engineering

Newton-Raphson Method

- It is perhaps the most widely used of all root-locating method.
- If the initial guess at the root is x_i , a tangent can be extended from the point $[x_i, f(x_i)]$.
- The point where this tangent crosses the x axis usually represents an improved estimate of the root.

Bangladesh University of Eng. & Tech. Slide 19 of 62 Industrial & Production Engineering

Newton-Raphson Method

- The Newton-Raphson method can be derived on the basis of this **geometrical interpretation**.

$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}}$$

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

Newton-Raphson formula

Bangladesh University of Eng. & Tech. Slide 20 of 62 Industrial & Production Engineering

Example 3

Problem Statement. Use the Newton-Raphson method to estimate the root of $f(x) = e^{-x} - x$ employing an initial guess of $x_0 = 0$.

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

$$x_{i+1} = x_i - \frac{e^{-x_i} - x_i}{-e^{-x_i} - 1}$$

| i | x_i | $ e_i , \%$ |
|-----|--------------|-------------|
| 0 | 0 | 100 |
| 1 | 0.5000000000 | 11.8 |
| 2 | 0.566311003 | 0.147 |
| 3 | 0.567143165 | 0.0000220 |
| 4 | 0.567143290 | $< 10^{-5}$ |

Bangladesh University of Eng. & Tech. Slide 21 of 62 Industrial & Production Engineering

Derivation and Error Analysis of Newton-Raphson Method

- Newton-Raphson method may also be developed from the Taylor series expansion.
- This alternative derivation is useful in that it also provides insight into the **rate of convergence** of the method.

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(\xi)}{2!}(x_{i+1} - x_i)^2$$

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

Bangladesh University of Eng. & Tech. Slide 22 of 62 Industrial & Production Engineering

Derivation and Error Analysis of Newton-Raphson Method

- At the intersection with the x axis, $f(x_{i+1})$ would be equal to zero.

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

$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

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

Bangladesh University of Eng. & Tech. Slide 23 of 62 Industrial & Production Engineering

Derivation and Error Analysis of Newton-Raphson Method

- Taylor series can also be used to estimate the error of the formula.
- This can be done by realizing that if the complete Taylor series were employed, an exact result would be obtained.
- For this situation $x_{i+1} = x_r$, where x is the true value of the root.

$$0 = f(x_i) + f'(x_i)(x_r - x_i) + \frac{f''(\xi)}{2!}(x_r - x_i)^2$$

Bangladesh University of Eng. & Tech. Slide 24 of 62 Industrial & Production Engineering

Derivation and Error Analysis of Newton-Raphson Method

$$0 = f(x_i) + f'(x_i)(x_r - x_i) + \frac{f''(\xi)}{2!}(x_r - x_i)^2$$

$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

$$0 = f'(x_i)(x_r - x_{i+1}) + \frac{f''(\xi)}{2!}(x_r - x_i)^2$$

$$E_{i,i+1} = x_r - x_{i+1}$$

$$0 = f'(x_i)E_{i,i+1} + \frac{f''(\xi)}{2!}E_{i,i}^2$$

Bangladesh University of Eng. & Tech.
Slide 25 of 62
Industrial & Production Engineering

Derivation and Error Analysis of Newton-Raphson Method

$$0 = f'(x_i)E_{i,i+1} + \frac{f''(\xi)}{2!}E_{i,i}^2$$

- If we assume convergence, both x_i and ξ should eventually be approximated by the root x_r .

$$E_{i,i+1} = \frac{-f''(x_r)}{2f'(x_r)}E_{i,i}^2$$

- The error is roughly proportional to the square of the previous error.
- This means that the number of correct decimal places approximately doubles with each iteration.
- Such behavior is referred to as **quadratic convergence**.

Bangladesh University of Eng. & Tech.
Slide 26 of 62
Industrial & Production Engineering

Termination Criteria and Error Estimates

$$\varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| 100\%$$

- The Taylor series derivation of the method provides theoretical insight regarding the rate of convergence as expressed by $E_{i+1} = O(E_i^2)$.
- Thus the error should be roughly proportional to the square of the previous error.
- In other words, the number of significant figures of accuracy approximately doubles with each iteration.
- This behavior is called **quadratic convergence** and is one of the major reasons for the popularity of the method.

Bangladesh University of Eng. & Tech.
Slide 27 of 62
Industrial & Production Engineering

Example 4

Problem Statement. Use the Newton-Raphson method to estimate the root of $f(x) = e^{-x} - x$ employing an initial guess of $x_0 = 0$.

$$E_{i,i+1} \cong \frac{-f''(x_r)}{2f'(x_r)}E_{i,i}^2$$

Examine this formula and see if it applies to the results of Example 6.3.

Bangladesh University of Eng. & Tech.
Slide 28 of 62
Industrial & Production Engineering

Example 4

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

$$x_{i+1} = x_i - \frac{e^{-x_i} - x_i}{-e^{-x_i} - 1}$$

$x_r = 0.56714329$ $f'(0.56714329) = -1.56714329$

$f''(x) = e^{-x}$ $f''(0.56714329) = 0.56714329$

$$E_{i,i+1} \cong -\frac{0.56714329}{2(-1.56714329)}E_{i,i}^2 = 0.18095E_{i,i}^2$$

$E_{i,0} = 0.56714329$, $E_{i,1} \cong 0.18095(0.56714329)^2 = 0.0582$

Bangladesh University of Eng. & Tech.
Slide 29 of 62
Industrial & Production Engineering

Pitfalls of Newton-Raphson Method

- Although the Newton-Raphson method is often very efficient, there are situations where it performs poorly.
- A special case—multiple roots—will be addressed later.
- However, even when dealing with simple roots, difficulties can also arise, as in the following example.

Bangladesh University of Eng. & Tech.
Slide 30 of 62
Industrial & Production Engineering

Example 5

Problem Statement. Determine the positive root of $f(x) = x^{10} - 1$ using the Newton-Raphson method and an initial guess of $x = 0.5$.

| i | x_i | $ e_{a,i} , \%$ |
|-----|----------|-----------------|
| 0 | 0.5 | |
| 1 | 51.65 | 99.032 |
| 2 | 46.485 | 11.111 |
| 3 | 41.8365 | 11.111 |
| 4 | 37.65285 | 11.111 |
| ⋮ | | |
| 40 | 1.002316 | 2.130 |
| 41 | 1.000024 | 0.229 |
| 42 | 1 | 0.002 |

$$x_{i+1} = x_i - \frac{x_i^{10} - 1}{10x_i^9}$$

Convergence is very slow

Bangladesh University of Eng. & Tech.
Slide 31 of 62
Industrial & Production Engineering

Why does this happen?

- Notice how the first guess is in a region where the slope is near zero.
- Thus, the first iteration flings the solution far away from the initial guess to a new value ($x = 51.65$) where $f(x)$ has an extremely high value.

Bangladesh University of Eng. & Tech.
Slide 32 of 62
Industrial & Production Engineering

Pitfalls of Newton-Raphson Method (Cont'd)

- Aside from slow convergence due to the nature of the function, other difficulties can arise.

- An inflection point [i.e., $f''(x) = 0$] occurs in the vicinity of a root.
- Notice that iterations beginning at x_0 progressively diverge from the root.

Bangladesh University of Eng. & Tech.
Slide 33 of 62
Industrial & Production Engineering

Pitfalls of Newton-Raphson Method (Cont'd)

- It illustrates the tendency of the Newton-Raphson technique to oscillate around a local maximum or minimum.
- Such oscillations may persist, or, as in the fig., a near-zero slope is reached whereupon the solution is sent far from the area of interest.

Bangladesh University of Eng. & Tech.
Slide 34 of 62
Industrial & Production Engineering

Pitfalls of Newton-Raphson Method (Cont'd)

- It shows how an initial guess that is close to one root can jump to a location several roots away.
- This tendency to move away from the area of interest is because near-zero slopes are encountered.

Bangladesh University of Eng. & Tech.
Slide 35 of 62
Industrial & Production Engineering

Pitfalls of Newton-Raphson Method (Cont'd)

- A zero slope [$f'(x) = 0$] is truly a disaster because it causes division by zero in the Newton-Raphson formula.
- Graphically, it means that the solution shoots off horizontally and never hits the x axis.

Bangladesh University of Eng. & Tech.
Slide 36 of 62
Industrial & Production Engineering

Pitfalls of Newton-Raphson Method (Cont'd)

- Thus, there is no general convergence criterion for Newton-Raphson.
- Its convergence depends on the **nature of the function** and on the **accuracy of the initial guess**.
- The **only remedy** is to have an initial guess that is "sufficiently" close to the root. (for some functions, no guess will work!)
- Good guesses are usually predicated on **knowledge of the physical problem** setting or on devices such as **graphs** that provide insight into the behavior of the solution.
- The lack of a general convergence criterion also suggests that good computer software should be designed to recognize slow convergence or divergence.

Bangladesh University of Eng. & Tech.

Slide 37 of 62

Industrial & Production Engineering

Algorithm for Newton-Raphson

```

FUNCTION newtraph(x0, es, imax, iter, ea)
  xr = x0
  iter = 0
  DO
    xrold = xr
    xr = xr - func(xr)/dfunc(xr)
    iter = iter + 1
    IF xr ≠ 0 THEN
      ea = | (xr - xrold) / xr | * 100
    END IF
    IF ea < es OR iter ≥ imax EXIT
  END DO
  newtraph = xr
END newtraph

```

Bangladesh University of Eng. & Tech.

Slide 38 of 62

Industrial & Production Engineering

Algorithm for Newton-Raphson

- The program should incorporate several additional features:
 1. A plotting routine should be included in the program.
 2. At the end of the computation, the final root estimate should always be substituted into the original function to compute **whether the result is close to zero**. This check partially guards against those cases where slow or oscillating convergence may lead to a small value of ϵ_n while the solution is still far from a root.
 3. The program should always include **an upper limit on the number of iterations** to guard against oscillating, slowly convergent, or divergent solutions that could persist interminably.
 4. The program should alert the user and take account of the possibility that $f(x)$ might equal zero at any time during the computation.

Bangladesh University of Eng. & Tech.

Slide 39 of 62

Industrial & Production Engineering

Secant Method

- A potential problem in implementing the Newton Raphson method is the evaluation of the derivative.
- There are certain functions whose derivatives may be extremely difficult or inconvenient to evaluate.
- For these cases, the derivative can be approximated by a **backward finite divided difference**:

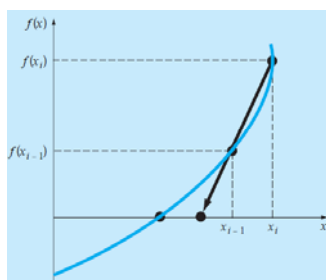
$$f'(x_i) \cong \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}$$

Bangladesh University of Eng. & Tech.

Slide 40 of 62

Industrial & Production Engineering

Secant Method



Bangladesh University of Eng. & Tech.

Slide 41 of 62

Industrial & Production Engineering

Secant Method

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

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

- This is the **formula for the secant method**.
- Notice that the approach requires two initial estimates of x .
- However, because $f(x)$ is not required to change signs between the estimates, it is not classified as a bracketing method.

Bangladesh University of Eng. & Tech.

Slide 42 of 62

Industrial & Production Engineering

Difference Between Secant and False-Position Methods

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

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

- A critical difference between the methods is how one of the initial values is replaced by the new estimate.
- Recall that in the false-position method the latest estimate of the root replaces whichever of the original values yielded a function value with the same sign as $f(x_i)$.
- Consequently, the two estimates always bracket the root. Therefore, for all practical purposes, the method always converges because the root is kept within the bracket.

Bangladesh University of Eng. & Tech.
Slide 43 of 62
Industrial & Production Engineering

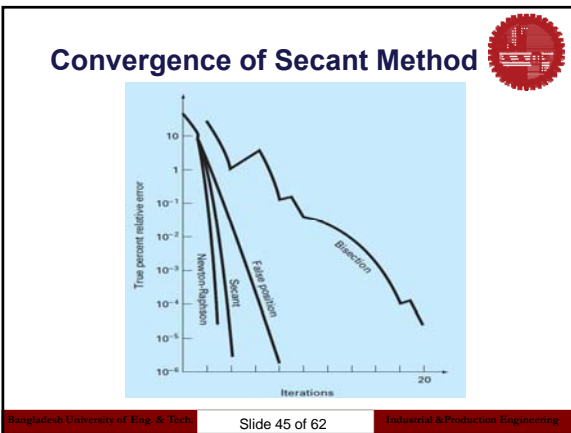
Difference Between Secant and False-Position Methods

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

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

- In contrast, the secant method replaces the values in strict sequence, with the new value x_{i+1} replacing x_i and x_i replacing x_{i-1} .
- As a result, the two values can sometimes lie on the same side of the root.
- For certain cases, this can lead to divergence.

Bangladesh University of Eng. & Tech.
Slide 44 of 62
Industrial & Production Engineering



Convergence of Secant Method

- Although the secant method may be divergent, when it converges it usually does so at a quicker rate than the false-position method.
- The inferiority of the false-position method is due to one end staying fixed to maintain the bracketing of the root.
- This property, which is an advantage in that it prevents divergence, is a shortcoming with regard to the rate of convergence.

Bangladesh University of Eng. & Tech.
Slide 46 of 62
Industrial & Production Engineering

Modified Secant Method

- Rather than using two arbitrary values to estimate the derivative, an alternative approach involves a **fractional perturbation** of the independent variable to estimate $f'(x)$:

$$f'(x_i) \approx \frac{f(x_i + \delta x_i) - f(x_i)}{\delta x_i}$$
- where δ = a small perturbation fraction.

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

Bangladesh University of Eng. & Tech.
Slide 47 of 62
Industrial & Production Engineering

Modified Secant Method

- The choice of a proper value for δ is not automatic.
- If δ is too small, the method can be swamped by round-off error caused by subtractive cancellation in the denominator of the formula.
- If it is too big, the technique can become inefficient and even divergent.
- However, if chosen correctly, it provides a nice alternative for cases where evaluating the derivative is difficult and developing two initial guesses is inconvenient.

Bangladesh University of Eng. & Tech.
Slide 48 of 62
Industrial & Production Engineering

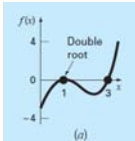
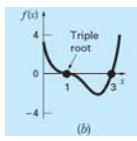
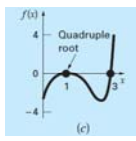
Modified Secant Method

- Further, in its most general sense, a **univariate function** is merely an entity that returns a single value in return for values sent to it.
- Perceived in this sense, functions are not always simple formulas like the one-line equations.
- For example, a function might consist of many lines of code that could take a significant amount of execution time to evaluate.
- In some cases, the function might even represent an independent computer program.
- For such cases, the secant and modified secant methods are valuable.

Bangladesh University of Eng. & Tech. Slide 49 of 62 Industrial & Production Engineering

Multiple Roots

- A multiple root corresponds to a point where a function is tangent to the x axis.

- In general, odd multiple roots cross the axis, whereas even ones do not.

Bangladesh University of Eng. & Tech. Slide 50 of 62 Industrial & Production Engineering

Multiple Roots

- Multiple roots pose some difficulties for many of the numerical methods discussed:
 - The fact that the function does not change sign at even multiple roots precludes the use of the reliable bracketing methods.
 - Another possible problem is related to the fact that not only $f(x)$ but also $f'(x)$ goes to zero at the root.
 - This poses problems for both the Newton-Raphson and secant methods, which both contain the derivative (or its estimate) in the denominator of their respective formulas.
 - This could result in division by zero when the solution converges very close to the root.
 - A simple way to circumvent these problems is based on the fact that it can be demonstrated theoretically (Ralston and Rabinowitz, 1978) that $f(x)$ will always reach zero before $f'(x)$.
 - Therefore, if a zero check for $f(x)$ is incorporated into the computer program, the computation can be terminated before $f(x)$ reaches zero.

Bangladesh University of Eng. & Tech. Slide 51 of 62 Industrial & Production Engineering

Multiple Roots

- It can be demonstrated that the Newton-Raphson and secant methods are linearly, rather than quadratically, convergent for multiple roots (Ralston and Rabinowitz, 1978).
 - Modifications have been proposed to alleviate this problem.
 - Ralston and Rabinowitz (1978) have indicated that a slight change in the formulation returns it to quadratic convergence, as in

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

- where m is the multiplicity of the root (that is, $m = 2$ for a double root, $m = 3$ for a triple root, etc.).
- This may be an unsatisfactory alternative because it hinges on foreknowledge of the multiplicity of the root.

Bangladesh University of Eng. & Tech. Slide 52 of 62 Industrial & Production Engineering

Multiple Roots

- Another alternative, also suggested by Ralston and Rabinowitz (1978), is to define a new function $u(x)$, that is, the ratio of the function to its derivative, as in

$$u(x) = \frac{f(x)}{f'(x)}$$
- It can be shown that this function has roots at all the same locations as the original function.

$$x_{i+1} = x_i - \frac{u(x_i)}{u'(x_i)} \quad u'(x) = \frac{f'(x)f''(x) - f(x)f'''(x)}{[f'(x)]^2}$$

$$x_{i+1} = x_i - \frac{f(x_i)f'(x_i)}{[f'(x_i)]^2 - f(x_i)f''(x_i)}$$

Bangladesh University of Eng. & Tech. Slide 53 of 62 Industrial & Production Engineering

Multiple Roots

- Although it is preferable for multiple roots, it is somewhat less efficient and requires more computational effort than the standard method for simple roots.
- It should be noted that a modified version of the secant method suited for multiple roots can also be developed.

$$u(x) = \frac{f(x)}{f'(x)}$$

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

Bangladesh University of Eng. & Tech. Slide 54 of 62 Industrial & Production Engineering

Systems of Nonlinear Equations

- Non-linear system of equations:

$$\begin{aligned} f_1(x_1, x_2, \dots, x_n) &= 0 \\ f_2(x_1, x_2, \dots, x_n) &= 0 \\ &\vdots \\ f_n(x_1, x_2, \dots, x_n) &= 0 \end{aligned}$$
- Most approaches for determining such solutions are extensions of the open methods for solving single equations.
- In this lecture, we will investigate two of these: **fixed-point iteration** and **Newton-Raphson**.

Bangladesh University of Eng. & Tech. Slide 55 of 62 Industrial & Production Engineering

Fixed-Point Iteration

Fixed-Point Iteration for a Nonlinear System

Problem Statement. Use fixed-point iteration to determine the roots of Eq. (6.19). Note that a correct pair of roots is $x = 2$ and $y = 3$. Initiate the computation with guesses of $x = 1.5$ and $y = 3.5$.

$$\begin{aligned} x^2 + xy &= 10 \\ \text{and} \\ y + 3xy^2 &= 57 \end{aligned}$$

$$x_{i+1} = \frac{10 - x_i^2}{y_i} \qquad x = \sqrt{10 - xy}$$

$$y_{i+1} = 57 - 3x_i y_i^2 \qquad y = \sqrt{\frac{57 - y}{3x}}$$

Bangladesh University of Eng. & Tech. Slide 56 of 62 Industrial & Production Engineering

Fixed-Point Iteration

- The previous example illustrates the most serious shortcoming of simple fixed-point iteration—that is, **convergence often depends on the manner in which the equations are formulated**.
- Additionally, even in those instances where convergence is possible, divergence can occur if the initial guesses are insufficiently close to the true solution.
- Using reasoning similar to that in Box 6.1, it can be demonstrated that sufficient conditions for convergence for the two-equation case are

$$\left| \frac{\partial u}{\partial x} \right| + \left| \frac{\partial u}{\partial y} \right| < 1 \qquad \left| \frac{\partial v}{\partial x} \right| + \left| \frac{\partial v}{\partial y} \right| < 1$$
- These criteria are so restrictive that fixed-point iteration has limited utility for solving nonlinear systems.
- However, it can be very useful for solving linear systems.

Bangladesh University of Eng. & Tech. Slide 57 of 62 Industrial & Production Engineering

Newton-Raphson

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

- This is the single-equation form of the Newton-Raphson method.
- The multiequation form is derived in an identical fashion.
- However, a multivariable Taylor series must be used to account for the fact that more than one independent variable contributes to the determination of the root.

Bangladesh University of Eng. & Tech. Slide 58 of 62 Industrial & Production Engineering

Newton-Raphson

$$u_{i+1} = u_i + (x_{i+1} - x_i) \frac{\partial u_i}{\partial x} + (y_{i+1} - y_i) \frac{\partial u_i}{\partial y}$$

and

$$v_{i+1} = v_i + (x_{i+1} - x_i) \frac{\partial v_i}{\partial x} + (y_{i+1} - y_i) \frac{\partial v_i}{\partial y}$$

- Just as for the single-equation version, the root estimate corresponds to the values of x and y , where u_{i+1} and v_{i+1} equal zero.

$$\begin{aligned} \frac{\partial u_i}{\partial x} x_{i+1} + \frac{\partial u_i}{\partial y} y_{i+1} &= -u_i + x_i \frac{\partial u_i}{\partial x} + y_i \frac{\partial u_i}{\partial y} \\ \frac{\partial v_i}{\partial x} x_{i+1} + \frac{\partial v_i}{\partial y} y_{i+1} &= -v_i + x_i \frac{\partial v_i}{\partial x} + y_i \frac{\partial v_i}{\partial y} \end{aligned}$$
- This is a set of two linear equations with two unknowns.

Bangladesh University of Eng. & Tech. Slide 59 of 62 Industrial & Production Engineering

Newton-Raphson

- Consequently, algebraic manipulations (for example, Cramer's rule) can be employed to solve for

$$\begin{aligned} x_{i+1} &= x_i - \frac{u_i \frac{\partial v_i}{\partial y} - v_i \frac{\partial u_i}{\partial y}}{\frac{\partial u_i}{\partial x} \frac{\partial v_i}{\partial y} - \frac{\partial u_i}{\partial y} \frac{\partial v_i}{\partial x}} \\ y_{i+1} &= y_i - \frac{u_i \frac{\partial v_i}{\partial x} - v_i \frac{\partial u_i}{\partial x}}{\frac{\partial u_i}{\partial x} \frac{\partial v_i}{\partial y} - \frac{\partial u_i}{\partial y} \frac{\partial v_i}{\partial x}} \end{aligned}$$
- The denominator of each of these equations is formally referred to as the determinant of the **Jacobian of the system**.

Bangladesh University of Eng. & Tech. Slide 60 of 62 Industrial & Production Engineering

Newton-Raphson



- Just as with fixed-point iteration, the Newton-Raphson approach will often diverge if the initial guesses are not sufficiently close to the true roots.
- Whereas graphical methods could be employed to derive good guesses for the single-equation case, no such simple procedure is available for the multiequation version.
- The two-equation Newton-Raphson approach can be generalized to solve n simultaneous equations.

Assignment-06



- Problems 6.3, 6.6, 6.12, 6.18, 6.26, 6.30.