ME 209
Numerical Methods

3. Finding Roots of the Equations:

Part II

Open Methods

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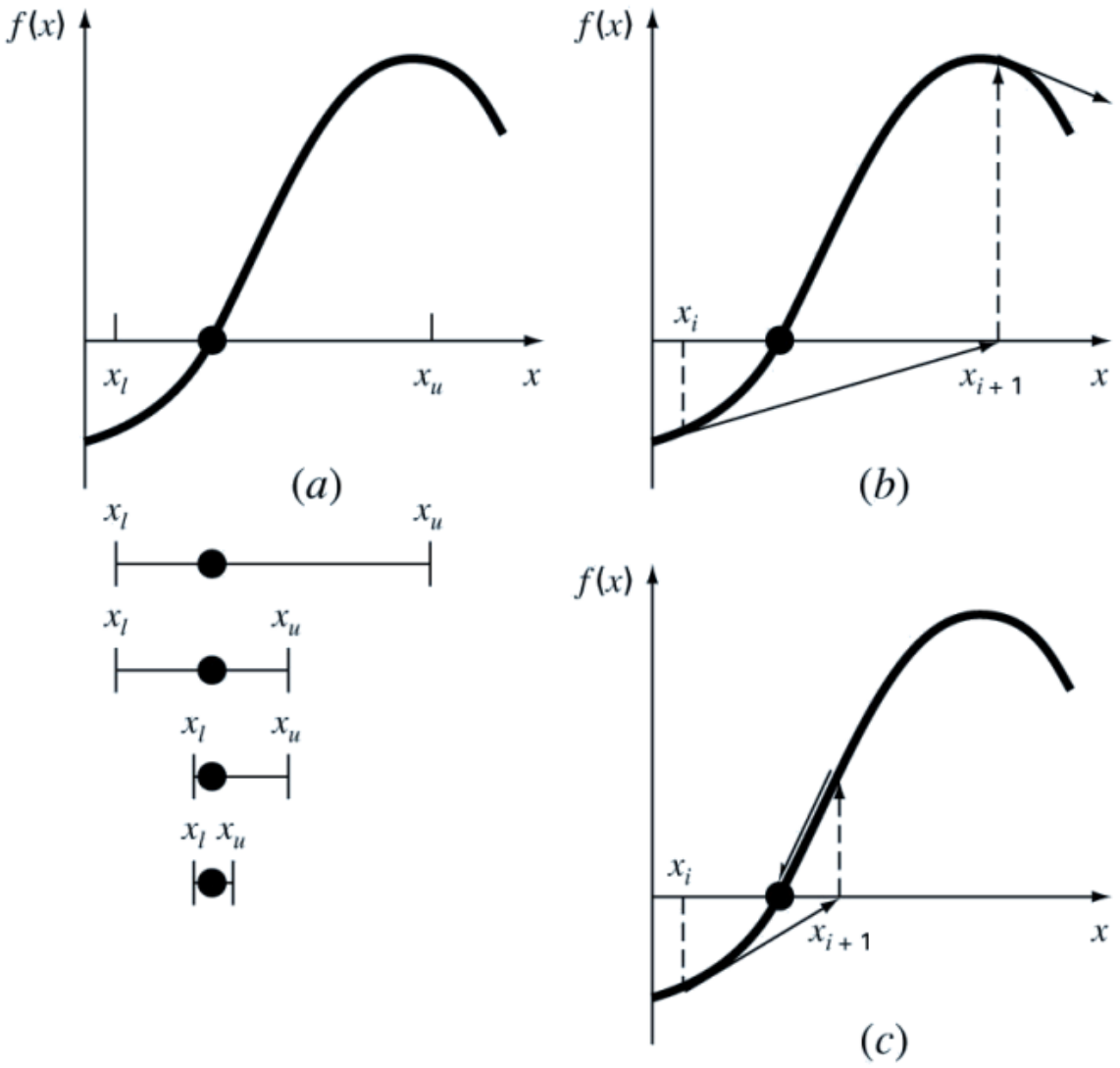
INTRODUCTION



- For the bracketing methods in previous part, the root is located within an interval prescribed by a lower and an upper bound.
- Repeated application of the bracketing methods always converges (figure a).
- In contrast, the *open methods* described in this part are based on *formulas* that require only a single starting value of *x* or two starting values that do not necessarily bracket the root.
- Thus, open methods may diverge (figure b) or converge very rapidly (figure c).

3.4 SIMPLE ONE-POINT ITERATION

In this method, the following procedure is applied:

1. Put the original formulation of *f(x) = 0* into a form of *x=g(x)* so that *x* is on the left-hand side of the equation.

Or, alternatively add x to both sides of the equation to yield into a form of *x=g(x).* For example:

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

Taking x on the left-hand side of the equation

$$\sin x = 0 \longrightarrow x = \sin x + x$$

Adding x on both side of the equation

2. Start with initial estimate x_i
3. Calculate a new estimate for the root using $x_{i+1} = g(x_i)$
4. As with the other iterative formulas, the approximate error for this equation can be determined using the error estimator:

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

5. Method converges if $|g'(x)| < 1$ in the region of interest.

Example:

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

$$f(x) = e^{-x} - x \longrightarrow x_{i+1} = e^{-x_i}$$

Starting with an initial guess of $x_0 = 0$, this iterative equation can be applied to compute

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

Checking the Possibility to Converge:

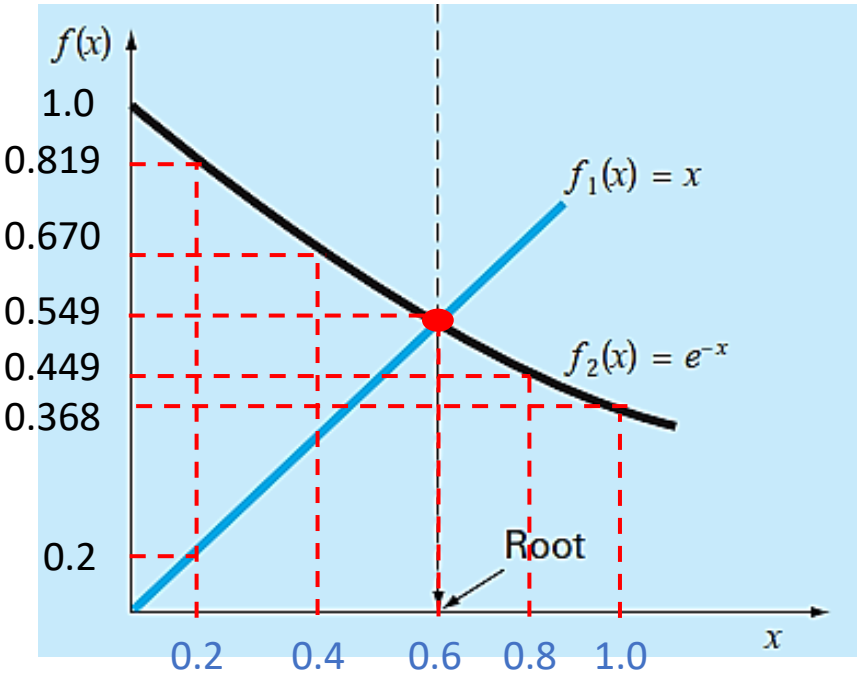
Let's check the convergency of the previous solution by applying two-curve graphical method. In this method, the function is separated into two component parts, as in

$$f_1(x) = f_2(x) \quad \text{where} \quad y_1 = f_1(x) \qquad y_2 = f_2(x)$$

The *x* values corresponding to the intersections of these functions represent the roots of $f(x) = 0$.

Reformulate the equation as $y_1 = x$ 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



The intersection of the two curves indicates a root estimate of approximately x = 0.57

Example:

Find the minimum positive root of the function.

$$f(x) = x^3 - x - 3 = 0$$

Solution: The given equation can be transformed into $x=g(x)$ in 3 different ways:

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

2) $x = \sqrt[3]{x+3} = g(x)$

3) $x = \frac{3}{x^2-1} = g(x)$

The results obtained when simple iteration is applied with all three equations by taking the initial value (x_i=1.5) are given in the table below.

Iteration (n)	$x_{i+1} = x_i^3 - 3$	$x_{i+1} = \sqrt[3]{x_i + 3}$	$x_{i+1} = \frac{3}{x_i^2 - 1}$
0	1.5	1.5	1.5
1	0.375	1.651	2.4
2	-2.947	1.669	0.63
3	-28.601	1.671	-4.974
4	-23399.241	1.672	0.126
5		1.672	-3.049
6			0.362
7			-3.452

- In the previous example, although the initial value is the same, it is seen that there is not always convergence and only one of the three states gives results.
- In other words, when the given function is written in the form x=g(x), it should be written in an appropriate manner, not randomly. Otherwise, convergence cannot be achieved, and a solution cannot be reached. The appropriate x=g(x) form is the form that satisfies the convergence criterion.
- Therefore, out of the three different expressions written above, only the second form that meets the convergence criterion gives results.

Convergence Criteria:

- If the real root (x_r) is written in the equation $x_{i+1} = g(x_i)$, the equation becomes $x_r = g(x_r)$.
- Then, two equations are subtracted side to side:

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

- If the right-hand side of this expression is multiplied and divided by the term $x_{i+1} - x_r$,and where x_s is a value between x_i and x_r.

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

$$= g'(x_s)(x_i - x_r)$$

From the mean value theorem,derivative of the function $g'(x_s)$

$$g'(x_s) = \frac{g(x_i) - g(x_r)}{x_i - x_r}$$

- And absolute error ε :

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

$$\varepsilon_{i+1} = g'(x_s).\varepsilon_i$$

- In order for convergence to occur, the error must decrease during the iteration. Thus in order to convergence,

$$|g'(x_s)| < 1$$

Example: Investigate the convergence criterion in the previous question.

The given equation was written as $x = g(x)$ in three different ways. In each case, let's take the derivative of the $g(x)$ function and examine it around the root.

1) $x = x^3 - 3$ $\quad g'(x) = 3x^2$ $\quad |g'(x_s)| > 1$

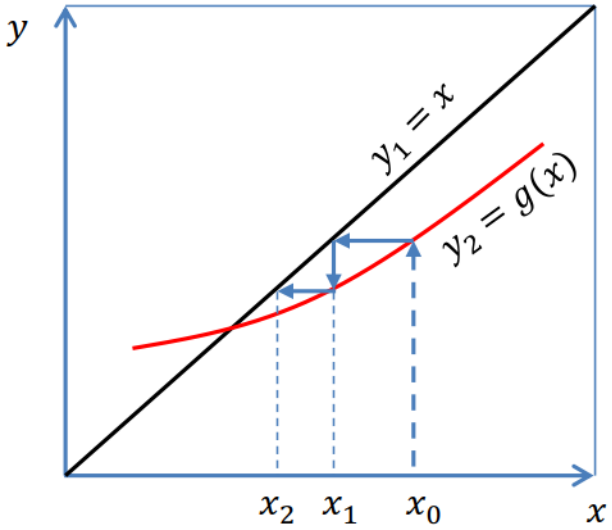
2) $x = \sqrt[3]{x+3}$ $\quad g'(x) = \frac{1}{3\sqrt[3]{(x+3)^2}}$ $\quad |g'(x_s)| < 1$

3) $x = \frac{3}{x^2-1}$ $\quad g'(x) = -\frac{6x}{(x^2-1)^2}$ $\quad |g'(x_s)| > 1$

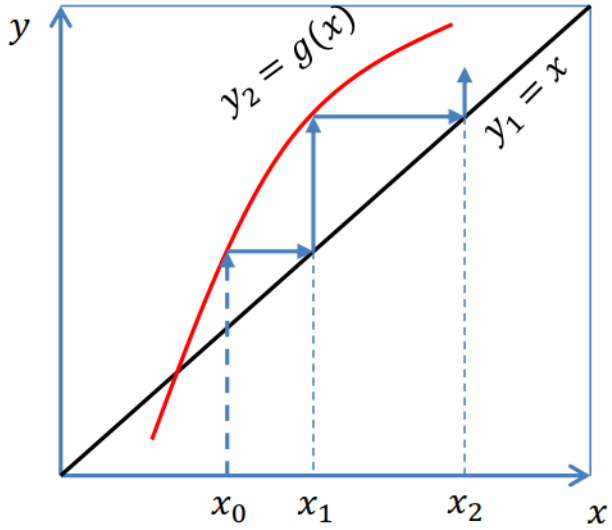
Only the second of these derivatives is always less than 1 for positive values of *x*. Therefore, the second way of writing definitely satisfies the convergence condition.

The first equation is always greater than one for $x > 0.58$, the last one is generally greater than one and less than one for some *x* values. Therefore, they should not be expected to yield results in simple iterations.

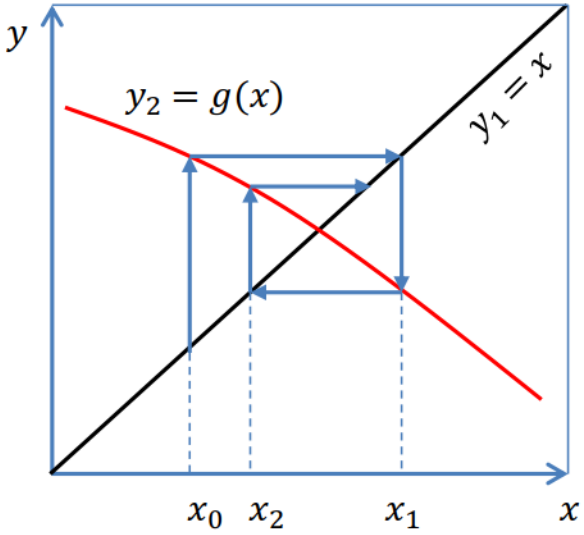
- We can use the two-curve graphical method to check convergence |g’(x)|<1.



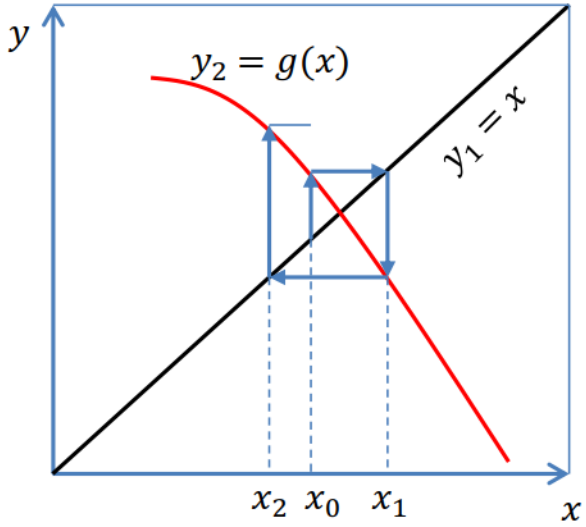
Monotone convergence



Monotone divergence



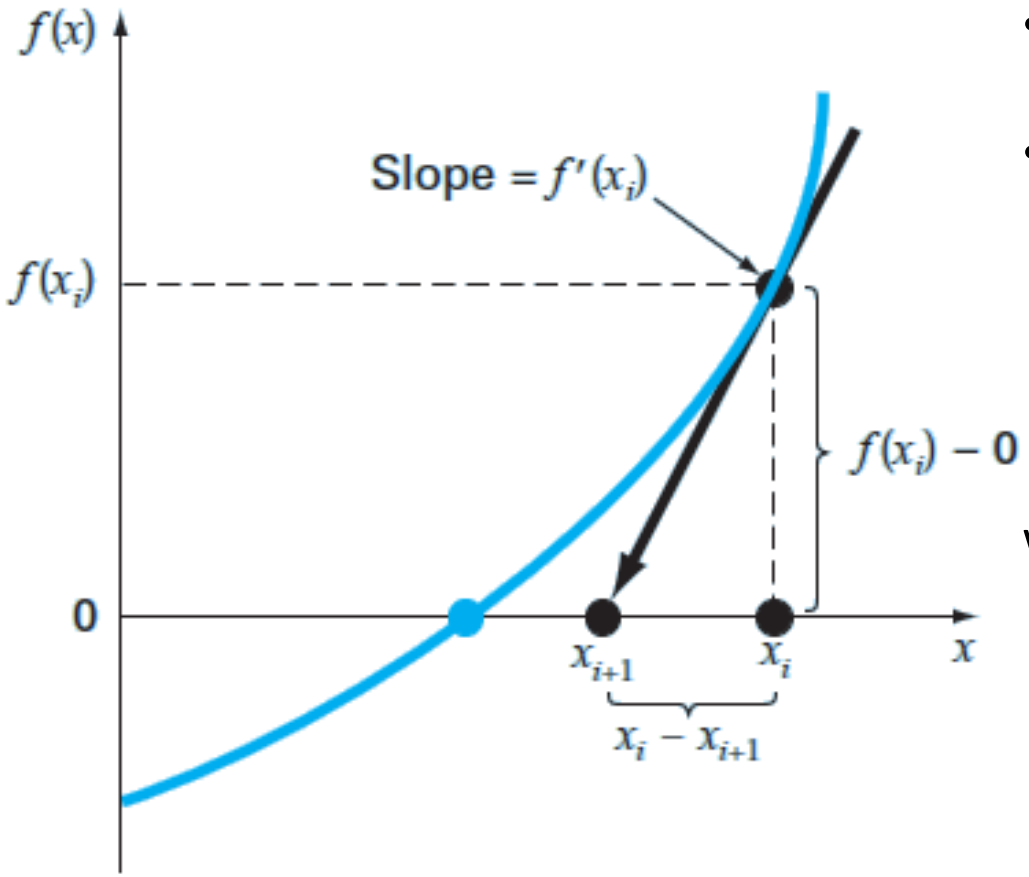
Spiral convergence



Spiral divergence

- The two-curve method can be used to illustrate the convergence and divergence of fixed-point iteration.
- First, equations can be re-expressed as a pair of equations y_1 =x and y_2 = g(x). These two equations can then be plotted separately.
- The roots of f(x)=0 correspond to the abscissa value at the intersection of the two curves.

3.5. Newton-Raphson Method



- The most widely used of all root-locating methods is the Newton-Raphson Method.
- The Newton-Raphson method can be derived on the basis of this geometrical interpretation. The first derivative at x is equivalent to the slope:

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

which can be rearrenged to yield

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

which is called the *Newton-Raphson formula.*

- As in the other root finding methods, percent relative error can be used as termination criteria. So, the iterative calculations is repeated until $|\varepsilon_a| < \varepsilon_s$

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

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

Starting with an initial guess of $x_0 = 0$, this iterative equation can be applied to compute

i	x_i	ε_t (%)
0	0	100
1	0.500000000	11.8
2	0.566311003	0.147
3	0.567143165	0.0000220
4	0.567143290	$< 10^{-8}$

Thus, the approach rapidly converges on the true root. Notice that the true percent relative error at each iteration decreases much faster than it does in simple fixed-point iteration

Example 2

Find the root of third order polynomial with an initial estimate of the root of 6.0

$$f(x) = x^3 - x^2 - 10x - 8$$

The derivative of this function is

$$f'(x) = 3x^2 - 2x - 10$$

The first trial estimate

$$x_1 = 6 - \frac{(6)^3 - (6)^2 - 10(6) - 8}{3(6)^2 - 2(6) - 10} = 6 - 1.3023 = 4.6977$$

Using this value as the revised estimate of x_1=4.6977, the second estimate

$$x_2 = 4.67977 - \frac{(4.6977)^3 - (4.6977)^2 - 10(4.6977) - 8}{3(4.6977)^2 - 2(4.6977) - 10}$$

$$= 4.6977 - 0.5688 = 4.1289$$

A third trial would yield an estimate of the root of 4.0057, and

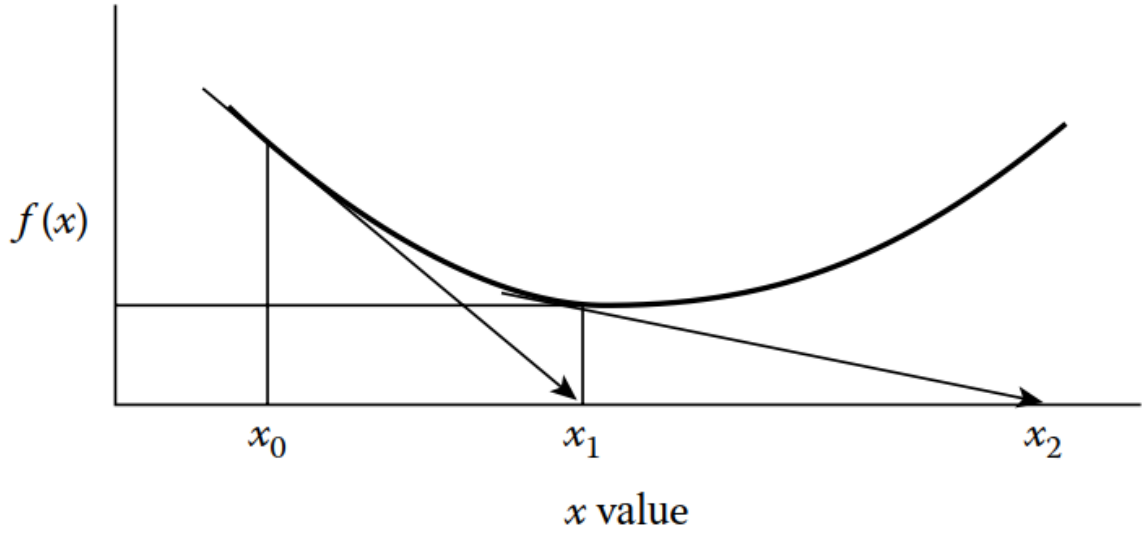
The fourth trial would yield a value of 4.0000

For precision to five significant digits, the value does not change with additional iterations·

NONCONVERGENCE

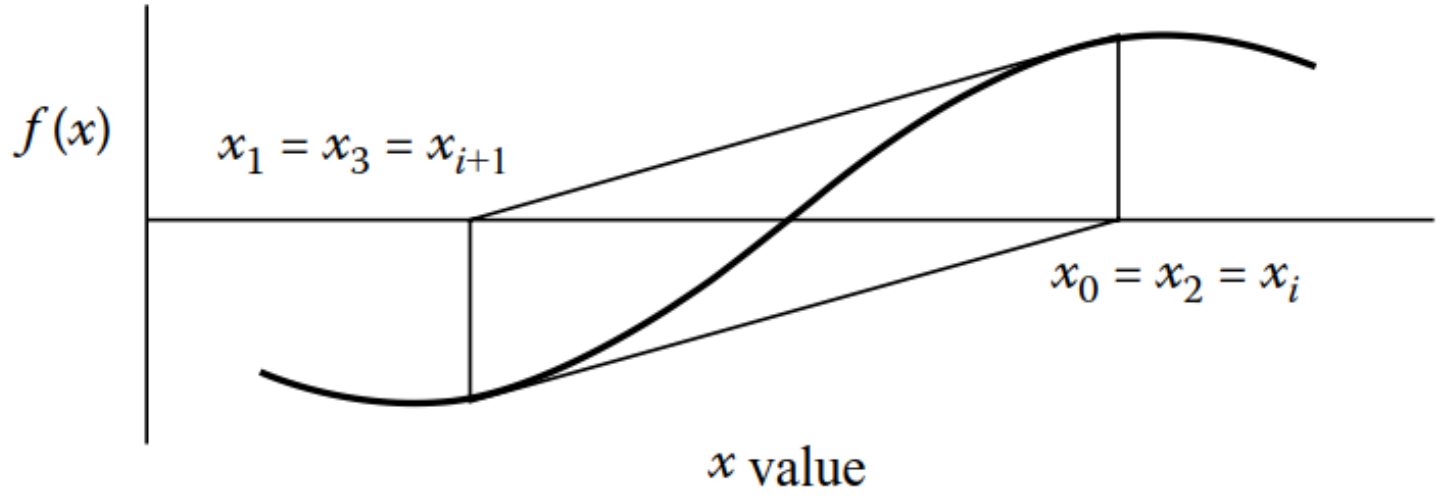
The Newton–Raphson iteration usually converges to a root faster than does the bisection method. However, this increase in speed does not come without liabilities; under certain circumstances, Newton–Raphson iteration may fail to converge.

If the initial estimate is selected such that the derivative of the function equals zero. $f(x_i)/f'(x_i)$ would equal infinity

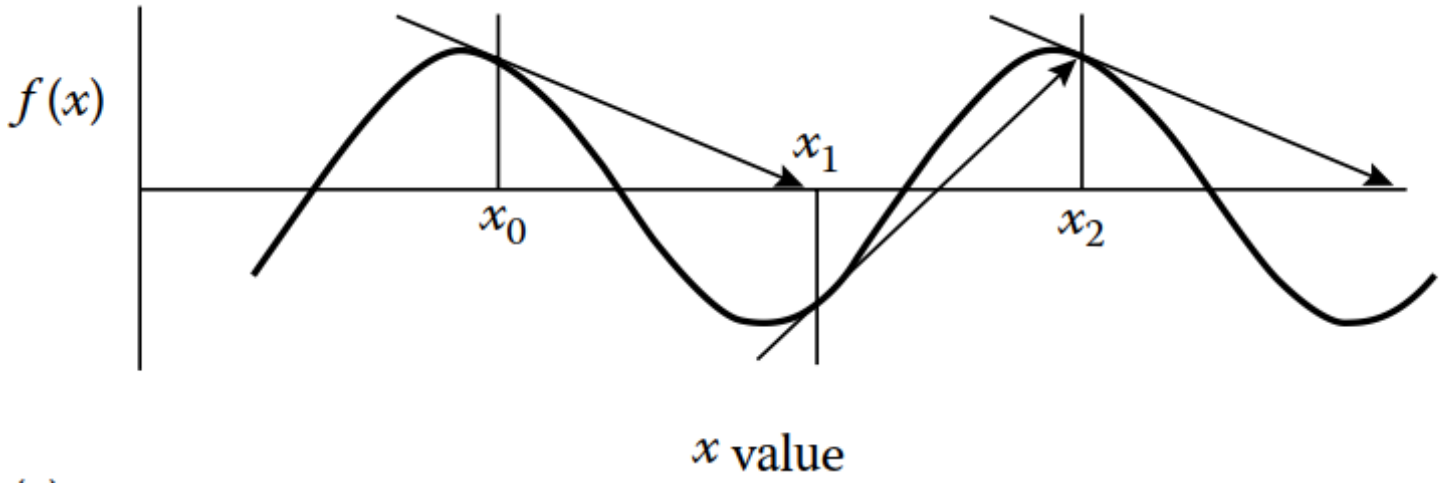


$f'(x_i)$ is approaching zero

A second instance of nonconvergence would occur if $f(x_i)/f'(x_i)$ equals $-f(x_{i+1})/f'(x_{i+1})$. In this case, x_i would equal x_{i+2} (where i is the iteration number) and x_{i+1} would equal x_{i+3} . Thus the solution would involve iterating between values of x_i and x_{i+1}

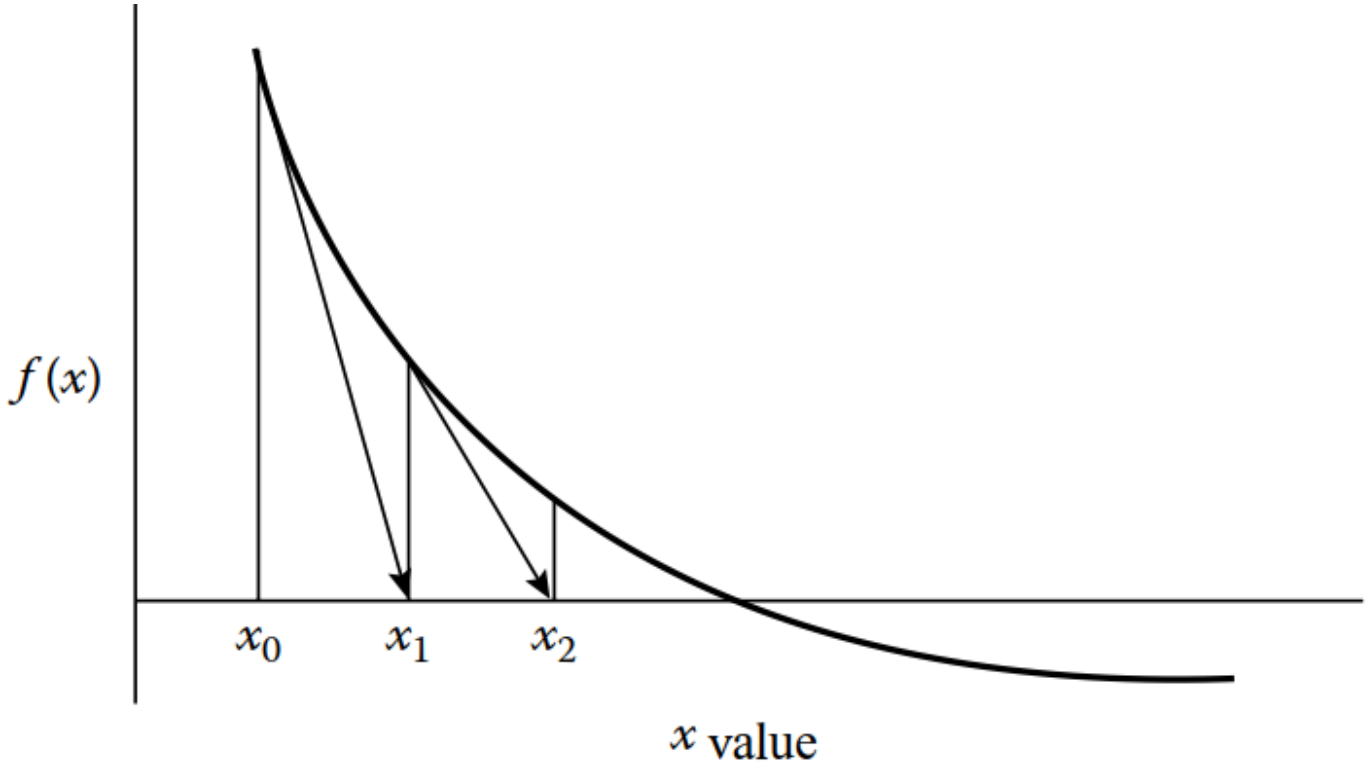


similarity of slopes



excessive iteration because of the periodic function

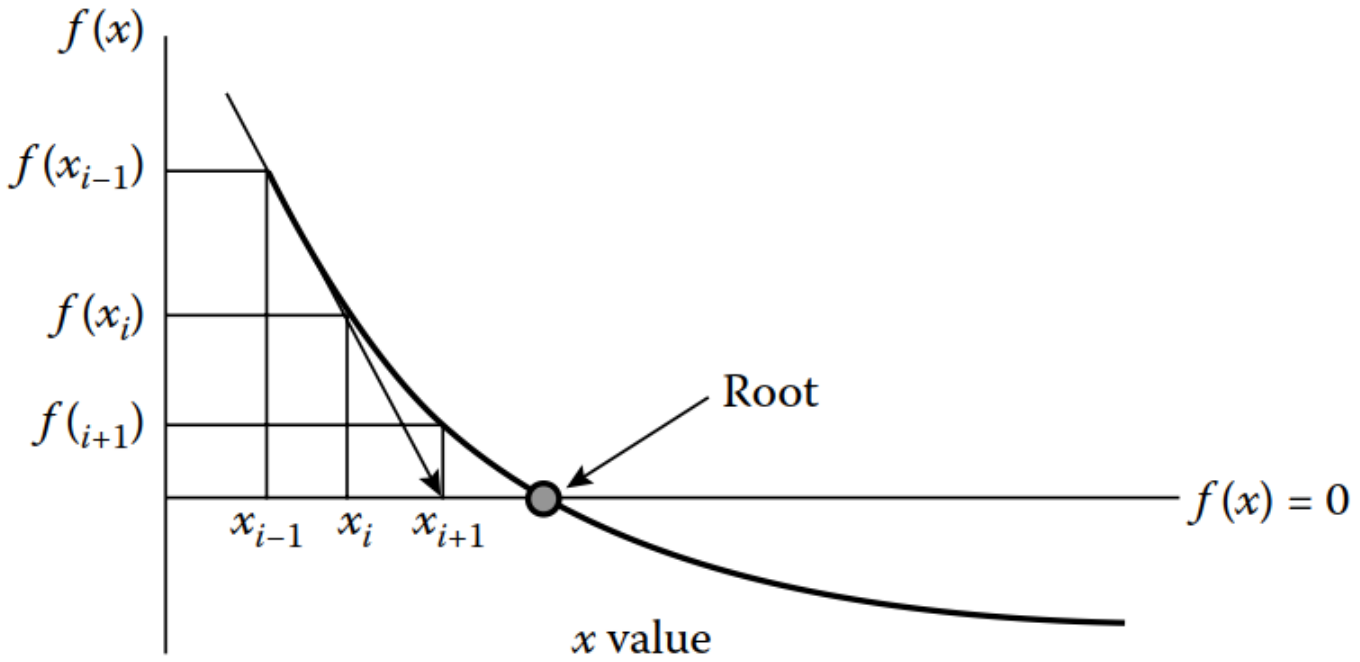
A large number of iterations will be required if the value of $f'(x_i)$ is much larger than $f(x_i)$.
In such cases, $f(x_i)/f'(x_i)$ is small, which leads to a small adjustment at each iteration.
This situation can occur, for example, when the root of a polynomial is near zero.



Excessive iteration because of the poor initial estimate

3.6. THE SECANT METHOD

A potential problem in implementing the Newton-Raphson method is the evaluation of the derivative. Although this is not inconvenient for polynomials and many other functions, 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:



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

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

Example. Use the secant method to estimate the root of $f(x) = e^{-x} - x$. Employ an initial estimates of $x_{-1}=0$ and $x_0=1.0$.

First iteration:

$$x_{-1} = 0 \qquad f(x_{-1}) = 1.00000$$

$$x_0 = 1 \qquad f(x_0) = -0.63212$$

$$x_1 = 1 - \frac{-0.63212(0-1)}{1-(-0.63212)} = 0.61270 \qquad \varepsilon_t = 8.0\%$$

Second iteration:

$$x_0 = 1 \qquad f(x_0) = -0.63212$$
$$x_1 = 0.61270 \qquad f(x_1) = -0.07081$$

(Note that both estimates are now on the same side of the root.)

$$x_2 = 0.61270 - \frac{-0.07081(1 - 0.61270)}{-0.63212 - (-0.07081)} = 0.56384 \qquad \varepsilon_t = 0.58\%$$

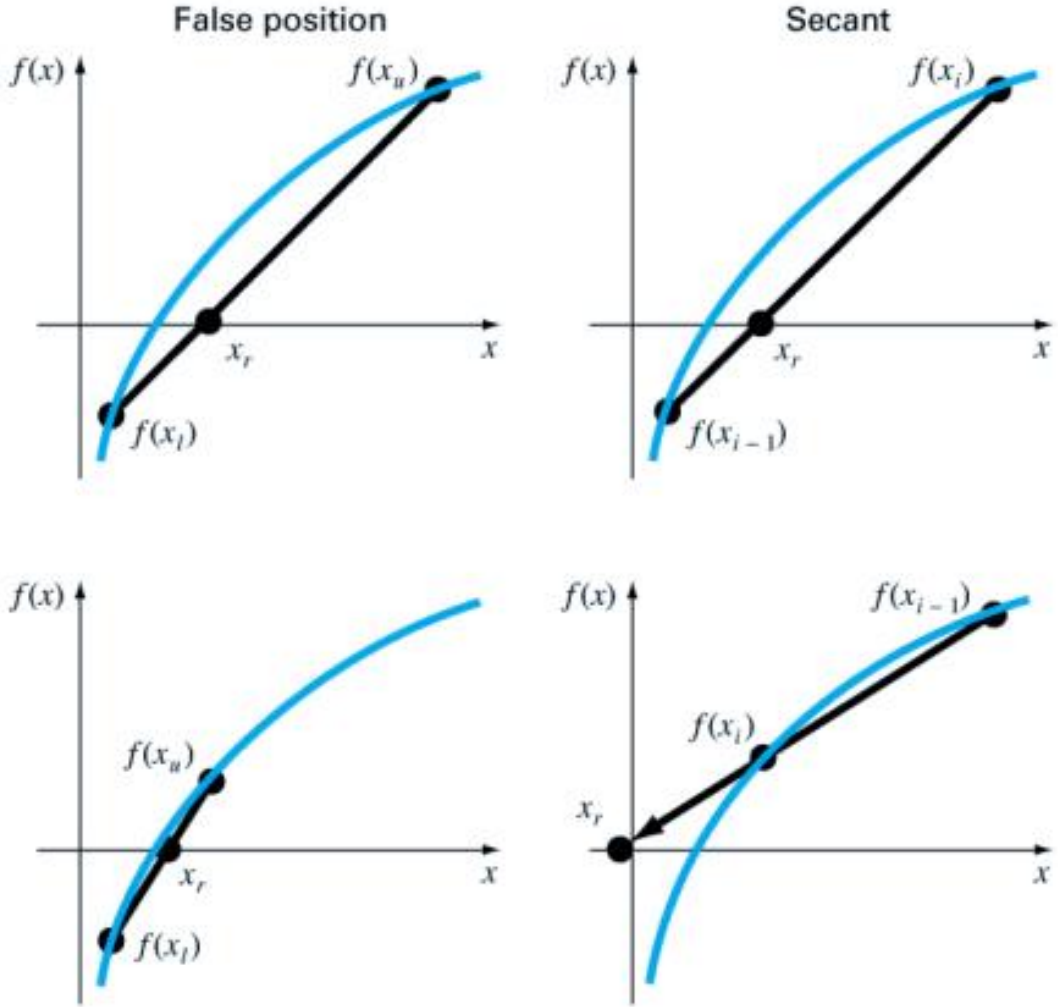
Third iteration:

$$x_1 = 0.61270 \qquad f(x_1) = -0.07081$$
$$x_2 = 0.56384 \qquad f(x_2) = 0.00518$$
$$x_3 = 0.56384 - \frac{0.00518(0.61270 - 0.56384)}{-0.07081 - (-0.00518)} = 0.56717 \qquad \varepsilon_t = 0.0048\%$$

3.6.1 Difference Between Secant and False-position Method

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

False-Position: $$x = x_U - \frac{f(x_U)(x_L - x_U)}{f(x_L) - f(x_U)}$$

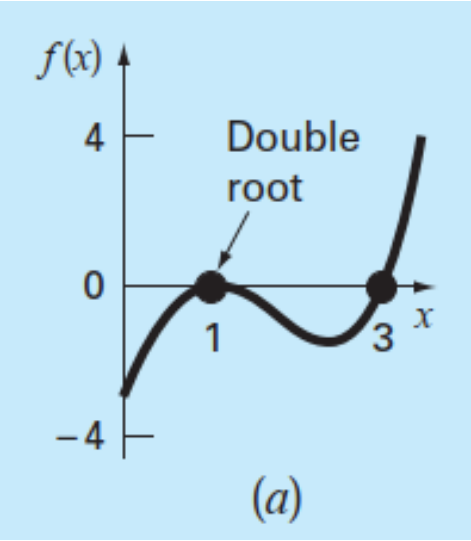


- First iterations of both methods are the same.
- Second iterations are different in terms of how the previous estimates are replaced with the newly calculated root.
- False-position Method drops one of previous estimates so that the remaining ones bracket the root.
- Secant Method always drops the oldest estimate.

3.7 Multiple Roots

A multiple root corresponds to a point where a function is tangent to the x axis. For example, a double root results from

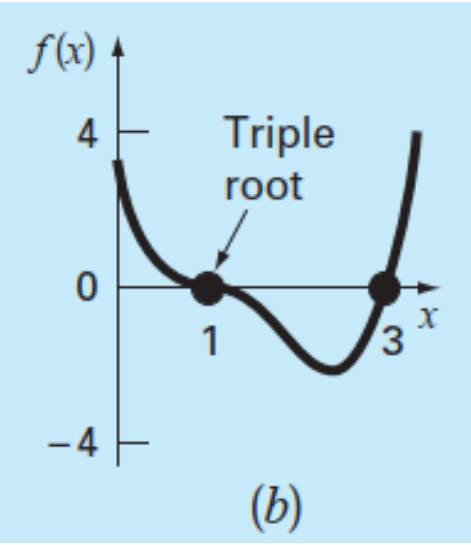
$$f(x) = (x - 3)(x - 1)(x - 1)$$



The equation has a *double root* because one value of *x* makes two terms. Graphically, this corresponds to the curve touching the x axis tangentially at the double root. Examine Fig. (a) at x = 1. Notice that the function touches the axis but does not cross it at the root.

A triple root corresponds to the case where one x value makes three terms in an equation equal to zero, as in

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



Notice that the graphical depiction (Fig. (b)) again indicates that the function is tangent to the axis at the root, but that for this case the axis is crossed. In general, odd multiple roots cross the axis, whereas even ones do not.

As summary:

1. The fact that the function does not change sign at even multiple roots precludes the use of the reliable bracketing methods that were discussed in previous lecture. Thus, of the methods covered in this course, you are limited to the open methods that may diverge.
2. 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.

   Some modifications can be made for this issue:

i) If you know the multiplicity of the root, Newton-Raphson formula can be modified as

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

m=2 for a double root, m=3 for a triple root, etc.

ii) Another alternative is to define a new function u(x)=f(x)/f‘(x) and use it in the formulation of Modified Newton Raphson Method (developed by Ralston and Rabinowitz 1978)

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

Example: Use both the standard and modified Newton-Raphson methods to evaluate the multiple root of following equation with an initial guess of $x_0 = 0$.

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

The first derivative of the equation $f'(x) = 3x^2 - 10x + 7$

In standart Newton-Raphson method:

$$x_{i+1} = x_i - \frac{x_i^3 - 5x_i^2 + 7x_i - 3}{3x_i^2 - 10x_i + 7}$$

By solving iteratively:

$$x_{i+1} = x_i - \frac{x_i^3 - 5x_i^2 + 7x_i - 3}{3x_i^2 - 10x_i + 7}$$

i	x_i	ε_t (%)
0	0	100
1	0.4285714	57
2	0.6857143	31
3	0.8328654	17
4	0.9133290	8.7
5	0.9557833	4.4
6	0.9776551	2.2

The method is linearly convergent toward the true value of 1.0.

For the modified method, the second derivative is

$$f''(x) = 6x - 10$$

$$x_{i+1} = x_i - \frac{(x_i^3 - 5x_i^2 + 7x_i - 3)(3x_i^2 - 10x_i + 7)}{(3x_i^2 - 10x_i + 7)^2 - (x_i^3 - 5x_i^2 + 7x_i - 3)(6x_i - 10)}$$

i	x_i	ε_t (%)
0	0	100
1	1.105263	11
2	1.003082	0.31
3	1.000002	0.00024

Thus, the modified formula is quadratically convergent.

3.8 SYSTEMS OF NONLINEAR EQUATIONS

To this point, we have focused on the determination of the roots of a single equation. A related problem is to locate the roots of a set of simultaneous equations,

$$\begin{aligned} f_1(x_1, x_2, \ldots, x_n) &= 0 \\ f_2(x_1, x_2, \ldots, x_n) &= 0 \\ \vdots & \quad \vdots \\ f_n(x_1, x_2, \ldots, x_n) &= 0 \end{aligned}$$

The solution of this system consists of a set of x values that simultaneously result in all the equations equaling zero.

3.8.1. Solving by Simple One-point Iteration

Example:

$$f_1(x,y) = x^2 + xy = 10$$
$$f_2(x,y) = y + 3xy^2 = 57$$

Solve the equations using the fixed-point iteration method and taking the initial values $x_0 = 1.5,\ y_0 = 3.5$

1. Solution: We leave one unknown in the given functions and write them as $x=g(x,y)$ and $y=h(x,y)$.

1. Iteration:

$$x_{i+1} = \frac{10 - x_i^2}{y_i} \qquad x = \frac{10 - (1.5)^2}{3.5} = 2.21429$$

$$y_{i+1} = 57 - 3x_i y_i^2 \qquad y = 57 - 3(2.21429)(3.5)^2 = -24.37516$$

2. Iteration:

$$x = \frac{10 - (2.21429)^2}{-24.37516} = -0.20910$$

$$y = 57 - 3(-0.20910)(-24.37516)^2 = 429.709$$

There appears to be divergence in the results. This is primarily due to the way we write the equations.

2. Solution: Let's write the equations $x=g(x,y)$ and $y=h(x,y)$ in a different format:

1. Iteration:

$$x = \sqrt{10 - xy} \qquad x = \sqrt{10 - 1.5(3.5)} = 2.17945$$

$$y = \sqrt{\frac{57 - y}{3x}} \qquad y = \sqrt{\frac{57 - 3.5}{3(2.17945)}} = 2.86051$$

2. Iteration:

$$x = \sqrt{10 - 2.17945(2.86051)} = 1.94053$$

$$y = \sqrt{\frac{57 - 2.86051}{3(1.94053)}} = 3.04955$$

Iterations are continued until the desired tolerance value is approached.

As can be seen from the example, convergence to root values in this method is highly dependent on the equation format and initial values chosen at the beginning. If the equations chosen at the beginning can satisfy the equations given below, convergence will occur.

$$\left|\frac{\partial f_1}{\partial x}\right| + \left|\frac{\partial f_1}{\partial y}\right| < 1$$

$$\left|\frac{\partial f_2}{\partial x}\right| + \left|\frac{\partial f_2}{\partial y}\right| < 1$$

3.8.2 Solving by Generalized Newton-Raphson Method

Let a nonlinear system with two unknowns, x and y, be given as follows.

$$f_1(x,y) = 0$$
$$f_2(x,y) = 0$$

$Jacobian\ matrix$

$$\begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = - \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$$

$$J(x_i, y_i).\Delta = -f_i \rightarrow \Delta = J^{-1}(x_i, y_i).-f_i$$

The values of Δx, Δy are obtained from the solution of the system of linear equations above. The roots of the equation are calculated according to these values as follows.

$$\Delta x = \frac{\frac{\partial f_1}{\partial y} f_2 - \frac{\partial f_2}{\partial y} f_1}{\frac{\partial f_1}{\partial x}\frac{\partial f_2}{\partial y} - \frac{\partial f_1}{\partial y}\frac{\partial f_2}{\partial x}} \qquad \Delta y = \frac{\frac{\partial f_2}{\partial x} f_1 - \frac{\partial f_1}{\partial x} f_2}{\frac{\partial f_1}{\partial x}\frac{\partial f_2}{\partial y} - \frac{\partial f_1}{\partial y}\frac{\partial f_2}{\partial x}}$$

$$x_{1,i+1} = x_{1,i} + \Delta x_1$$

$$y_{1,i+1} = y_{1,i} + \Delta y_1$$

Example:

$$f_1(x,y) = x^2 + xy = 10$$

$$f_2(x,y) = y + 3xy^2 = 57$$

Solve the equations using the Newton-Raphson method and using one iteration, taking the initial values $x_0 = 1.5,\ y_0 = 3.5$.

1.Iteration

$$\frac{\partial f_1}{\partial x} = \frac{\partial}{\partial x}(x^2 + xy - 10) = 2x + y = 6.5$$

$$\frac{\partial f_1}{\partial y} = \frac{\partial}{\partial y}(x^2 + xy - 10) = x = 1.5$$

$$\frac{\partial f_2}{\partial x} = \frac{\partial}{\partial x}(y + 3xy^2 - 57) = 3y^2 = 36.75$$

$$\frac{\partial f_2}{\partial y} = \frac{\partial}{\partial y}(y + 3xy^2 - 57) = 1 + 6xy = 32.5$$

$$f_1 = x^2 + xy - 10 = -2.5$$

$$f_2 = y + 3xy^2 - 57 = 1.625$$

$$\Delta x = \frac{\frac{\partial f_1}{\partial y} f_2 - \frac{\partial f_2}{\partial y} f_1}{\frac{\partial f_1}{\partial x}\frac{\partial f_2}{\partial y} - \frac{\partial f_1}{\partial y}\frac{\partial f_2}{\partial x}} = \frac{1.5 * 1.625 - 32.5 * -2.5}{6.5 * 32.5 - 1.5 * 36.75} = 0.53603$$

$$\Delta y = \frac{\frac{\partial f_2}{\partial x} f_1 - \frac{\partial f_1}{\partial x} f_2}{\frac{\partial f_1}{\partial x}\frac{\partial f_2}{\partial y} - \frac{\partial f_1}{\partial y}\frac{\partial f_2}{\partial x}} = \frac{36.75 * -2.5 - 6.5 * 1.625}{6.5 * 32.5 - 1.5 * 36.75} = -0.656125$$

$$x_1 = x_0 + \Delta x = 1.5 + 0.53603 = 2.03603$$

$$y_1 = y_0 + \Delta y = 3.5 + 0.656125 = 2.84388$$

NEXT WEEK
Solutions of Linear Equation Systems