MATH2089
Numerical Methods
Lecture 3

Nonlinear equations:

Bisection method,

Fixed point iteration,

Newton-Raphson method and

Secant method

Solving Nonlinear Equations

- For a number of equations, analytical solutions may be directly obtained from functions available on calculators and computers, such as in the form $y = ax^2 + bx + c = 0$

  For example, $y = x^2 - 3x + 2 = 0 \rightarrow (x - 1)(x - 2) = 0$
  The roots of x are 1 and 2 respectively

- In many engineering applications, many algebraic equations generally do not have analytical solutions

Examples

- Geometrical concentration factor in solar-energy collection

$$C = \frac{\pi (h / \cos A)^2 F}{0.5 \pi D^2 (1 + \sin A - 0.5 \cos A)}$$

where A is rim angle, F is fractional coverage, D is diameter of collector and h is height of collector. If C = 0.892, F = 0.8, D = 14.0, h = 300.0, determine A? Rearranging, we need to solve for

$$f(A) = \frac{72000\pi / (\cos A)^2}{98\pi (1 + \sin A - 0.5 \cos A)} - 1200 = 0$$

Examples (continue)

- Friction factor of suspension of fibrous particles

$$\frac{1}{\sqrt{f}} = \left(\frac{1}{k}\right)\ln\left(\mathrm{Re}\sqrt{f}\right) + \left(14 - \frac{5.6}{k}\right)$$

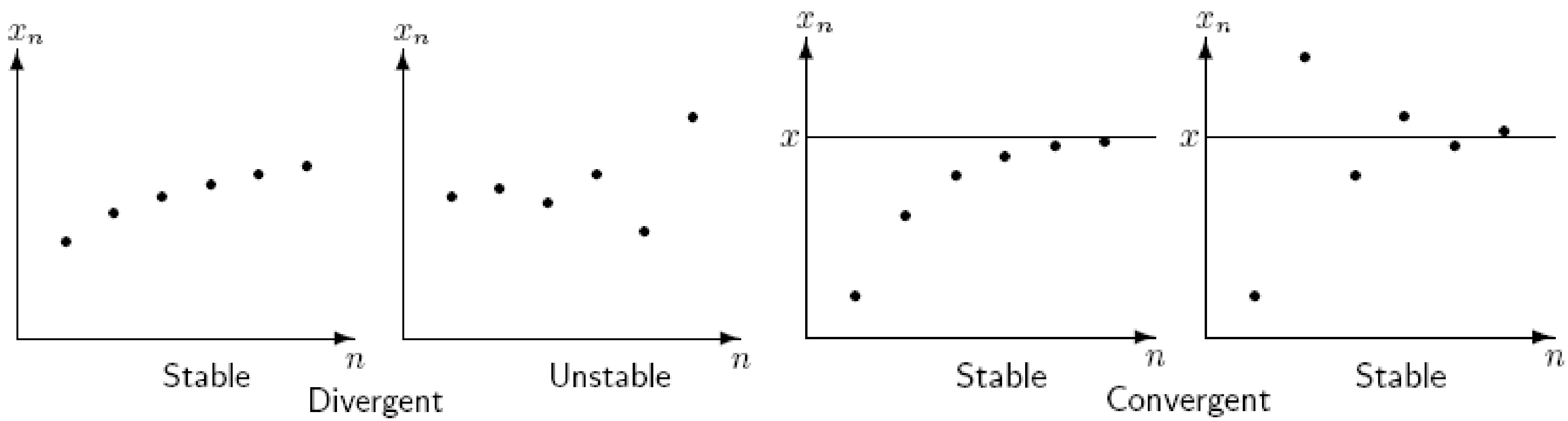
where Re is Reynolds number and k is a constant determined by the suspension concentration. For 0.8% concentration, k = 0.28. What is f when Re = 3500? Rearranging, we can solve for

$$g(f) = \frac{1}{\sqrt{f}} - \left(\frac{1}{0.28}\right)\ln\left(3750\sqrt{f}\right) - 7 = 0$$

Iterative Methods

- Such equations may be solved by seeking an *initial approximation* and improving this approximation using *iterative methods*
- If successive applications of the iterative method result in approximations which approach the solution, the iterative method is considered to be converged
- An appropriate *error estimate* is needed to detect if the method has ***converged*** sufficiently

Iterative Methods (continue)



- An iterative method may be inherently unstable or only for some initial approximations unstable
- A *correct, efficient and robust algorithm* requires an appropriate selection of both the approximate and iterative method

Useful Theorems

Taylor's Theorem

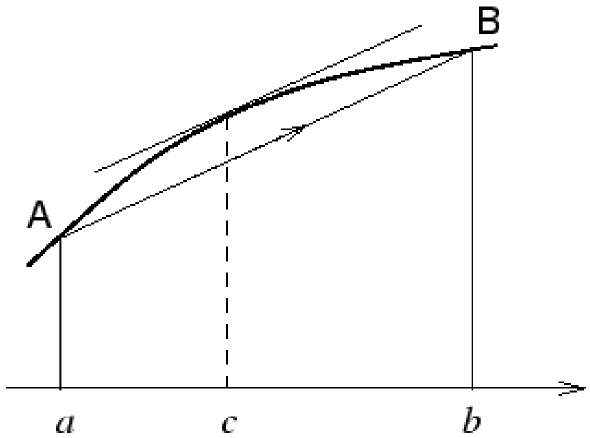
- Assume that the function *f(x)* and its derivatives are all continuous on [a, b]. If both x_0 and $x_0 + h$ lie in the interval [a, b] and $h = x - x_0$ then

$$f(x_0 + h) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!} h^k + O(h^{n+1})$$

is the n-th degree Taylor polynomial expansion of *f(x)* about x_0. Note that this theorem is very useful in deriving numerical methods!

Useful Theorems (continue)

Mean Value Theorem

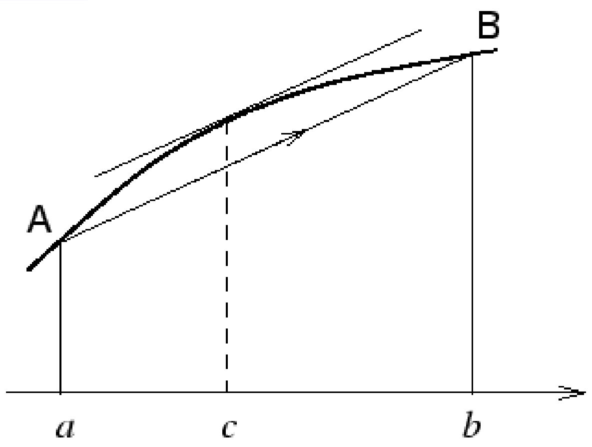


- Assume that $f \in C[a,b]$ and $f'(x)$ exists for all $x \in [a,b]$. Then there should exist a number c with $c \in [a,b]$ such that

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$

Useful Theorems (continue)

Mean Value Theorem



- Geometrically, the mean value theorem says that there is at least one number $c \in [a,b]$ such that the slope of the tangent line to the graph $y = f(x)$ at a point $\left(c, f(c)\right)$ equals the slope of secant line through the points $\left(a, f(a)\right)$ and $\left(b, f(b)\right)$

Initial Approximations

- Solutions are required within a given range and initial estimates can be found by
  - Random search
  - Systematic search, e.g. interval halving
  - Simplified equations
  - Graphical method

- For example, consider the following equation:

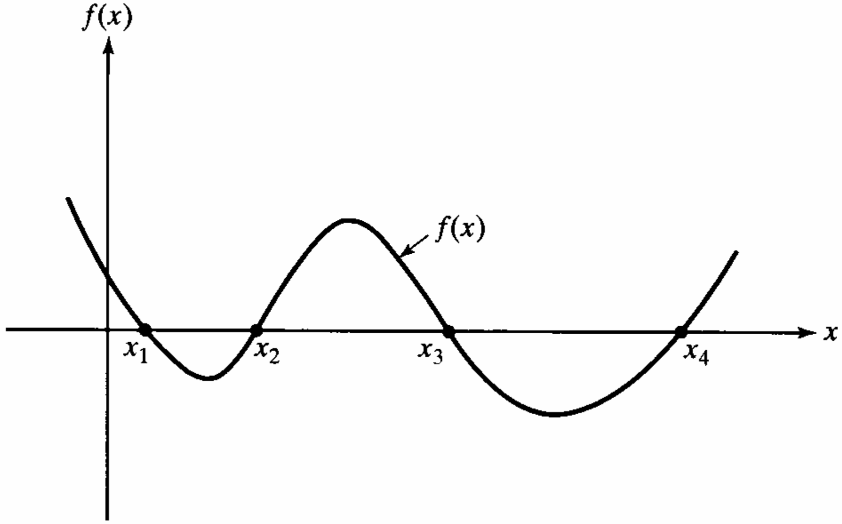
$$x^5 - x - 500 = 0$$

Initial estimate can be found by neglecting the middle term

$$x \approx 500^{1/5}$$

Initial Approximations (continue)

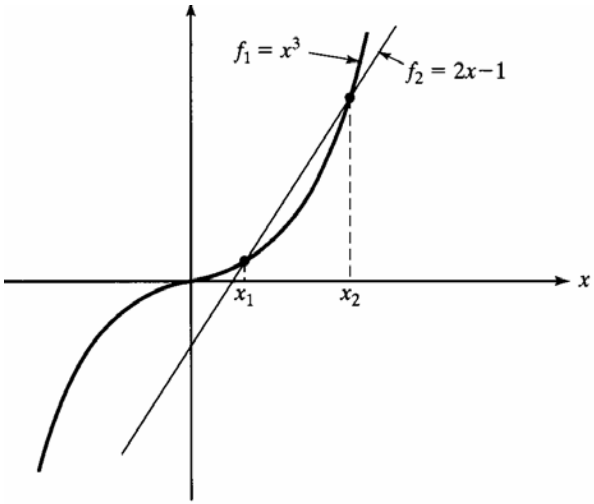
Graphical Method



- For the equation $x^5 - x - 500 = 0$, the root occurs when the function *f(x)* crosses the *x*-axis. It has four roots. Real root of an equation may be interpreted graphically except for complex equations

Initial Approximations (continue)

Graphical Method



- Split $f(x) = 0$ into two parts: $f(x) = f_1 - f_2 = 0 \rightarrow f_1 = f_2$ and the point of intersection of the two parts denotes the roots of the equation. The function is split into

$$f(x) = x^3 - (2x - 1) = f_1 - f_2$$

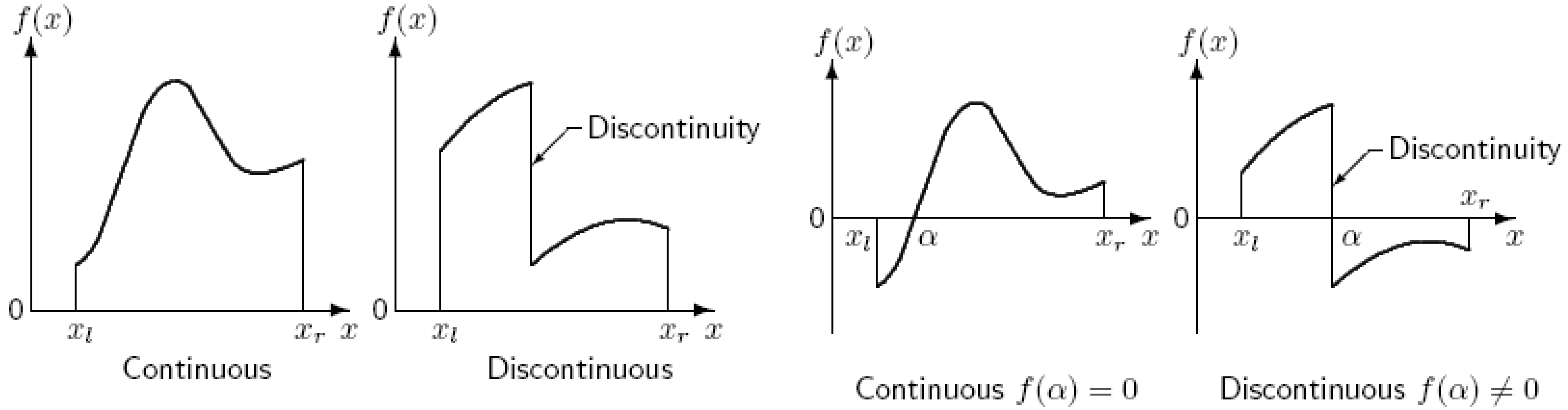
Initial Approximations (continue)

Graphical Method

- Usually used to find good starting points for other more accurate and efficient methods or to obtain rough estimates of roots!

Interval Halving (Bisection) Method

- Requires an initial range, $x_l < x < x_r$, with sign change so that $f(x_l)\, f(x_r) < 0$
- For each iteration, halve the interval, evaluate the function at the midpoint and make the new interval the half with a sign change
- Ensure the function is continuous as if the function is not continuous it may converge to a discontinuity



Interval Halving (Bisection) Method (continue)

- Initial estimate of the solution is

$$x_o = \left(x_l + x_r\right)/2$$

- Initial error is

$$E_i = \left|x_l - x_r\right|/2$$

and the number of iterations, *N*, required to reduce this error to E_r is

$$N = \log_2\left(\frac{E_i}{E_r}\right)$$

Steps of Solution

Step 1: Set a value of ε and choose the interval of uncertainty $(a^{(1)}, b^{(1)})$ that $f(a^{(1)}) \times f(b^{(1)}) < 0$ (Figure 1)

- Step 2: Compute $x_m^{(1)} = (a^{(1)} + b^{(1)})/2$
- Step 3: If $\left| f(x_m^{(1)}) \right| \le \varepsilon$, halt the procedure and get the estimated root as $x_m^{(1)}$, otherwise $\left| f(x_m^{(1)}) \right| > \varepsilon$, go to Step 4

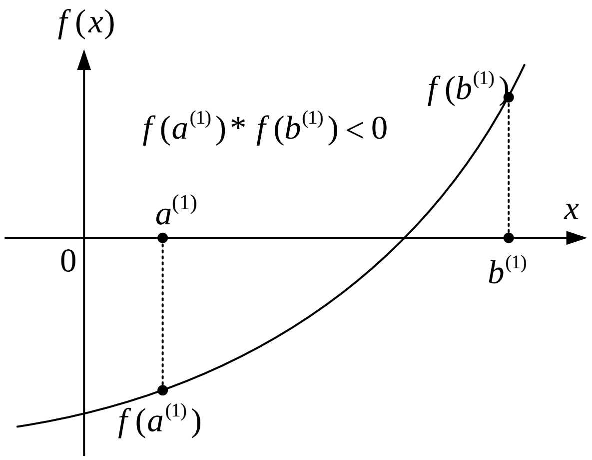


Figure 1

Steps of Solution (continue)

Step 4a: If $f(x_m^{(1)}) \times f(b^{(1)}) < 0$, set $(a^{(2)}, b^{(2)}) = (x_m^{(1)}, b^{(1)})$ (Figure 2) and go to Step 2

- Step 4b: If $f(x_m^{(1)}) \times f(b^{(1)}) > 0$, set $(a^{(2)}, b^{(2)}) = (a^{(1)}, x_m^{(1)})$ and go to Step 2
- Step 2: Compute $x_m^{(2)} = (a^{(2)} + b^{(2)})/2$
- Step 3: Check if $|f(x_m^{(2)})| \le \varepsilon$, answer = $x_m^{(2)}$, or $|f(x_m^{(1)})| > \varepsilon$ go to Step 4 to find a new interval $(a^{(3)}, b^{(3)})$

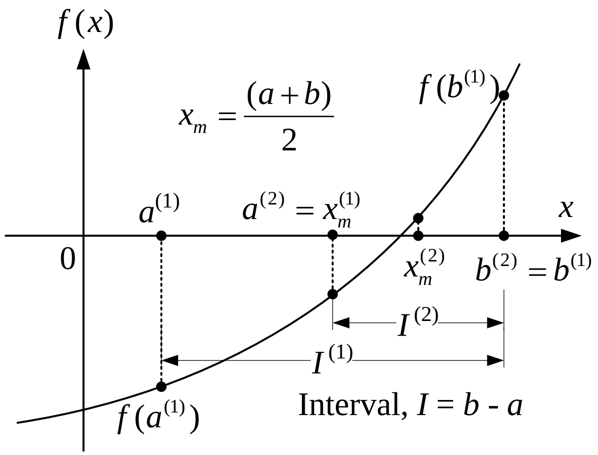


Figure 2

Convergence

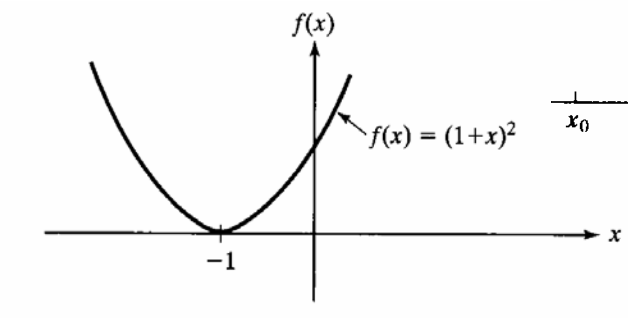
- The interval ($I = b - a$) is halved each time ($I^{(2)} = \frac{1}{2} I^{(1)}$), the last value of x_m differs from the root by less than $\frac{1}{2}$ the last interval

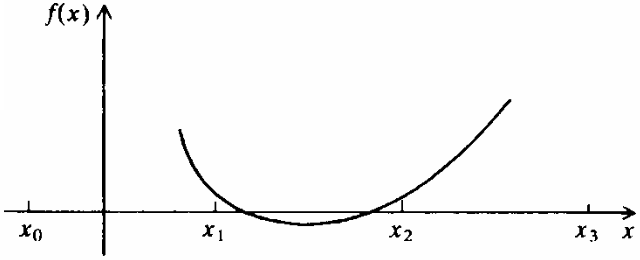
$$I^{(i+1)} = b^{(i+1)} - a^{(i+1)} = \frac{I^{(i)}}{2} = \frac{I^{(i-1)}}{2^2} = \frac{(b^{(1)} - a^{(1)})}{2^i}$$

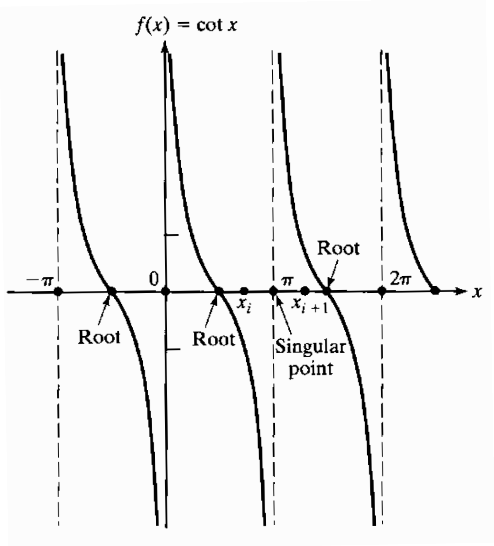
$$\text{Error after } i \text{ iterations} < \frac{(b^{(1)} - a^{(1)})}{2^i}$$

Convergence (continue)

- If the graph $f(x)$ of touches the x axis tangentially, $f(x)$ does not undergo a sign change, the method cannot find the root
- The bisection method will not work if the interval (a, b) contains a double root
- The method may not be able to distinguish between a singular point and a root







Convergence (continue)

- If $f(x)$ can be evaluated quickly, the bisection method is recommended
- The method cannot be used to find the complex roots of an equation

Example of Bisection Method

- Using the interval halving, a solution to $x^2 - 2 = 0$ is required between the roots 1 and 2

  - Show that the interval halving method will converge
  - Starting with this interval calculate the number of iterations required if the final error must be 0.02
  - Perform these iterations to obtain the answer to four significant figures

Fixed Point Iteration

- The function $f(x) = 0$ can be rewritten as $x = F(x)$ (or $x = g(x)$) to give an iterative procedure

$$x_{n+1} = F\left(x_n\right) \quad n = 1, 2, 3, \ldots$$

- This procedure may converge or diverge depending on the choice of $F(x)$. We can define the convergence criterion as

$$\left|x_{n+1} - x_n\right| \leq \varepsilon \quad \text{or} \quad \left|\frac{x_{n+1} - x_n}{x_{n+1}}\right| \leq \varepsilon$$

Convergence

- Based on $x_{n+1} = F(x_n)$, let S denote a solution and e_n the error in x_n so that $x_n = S + e_n$. Therefore,

$$S + e_{n+1} = F(S + e_n)$$

The right-hand side can be expanded in a Taylor series about S as

$$S + e_{n+1} = F(S)) + e_n F'(S) + \frac{e_n^2}{2!} F''(S) + \ldots$$

Since S is the solution, $S = F(S)$. Therefore,

$$e_{n+1} = e_n F'(S) + \frac{e_n^2}{2!} F''(S) + \ldots$$

Convergence (continue)

- If e_n is sufficiently small and provided that $F'(S) \neq 0$ then

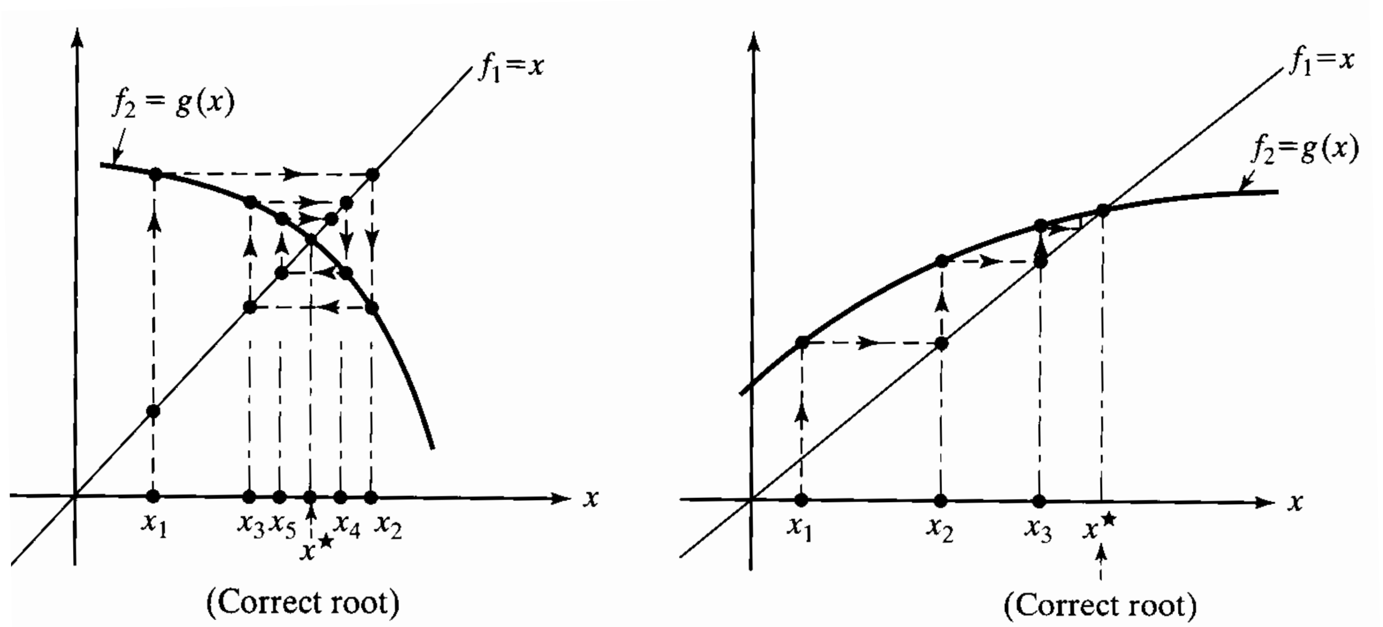
$$e_{n+1} \approx e_n F'(S)$$

For $x_{n+1} = F(x_n)$ to be convergent, it is necessary that $|e_{n+1}| < |e_n|$. It can be achieved if $|F'(S)| < 1$. Therefore, the iterative process is convergent if there is some range around S for which $|F'(S)| < R < 1$

Since $e_{n+1} < O(e_n)$, the fixed point iteration is a <u>first order method</u>, i.e. a fixed number of decimal places improvement in accuracy occurs at each iteration

Convergence (continue)

- Convergence criterion $|F'(S)| < R < 1$ possesses a simple geometric interpretation

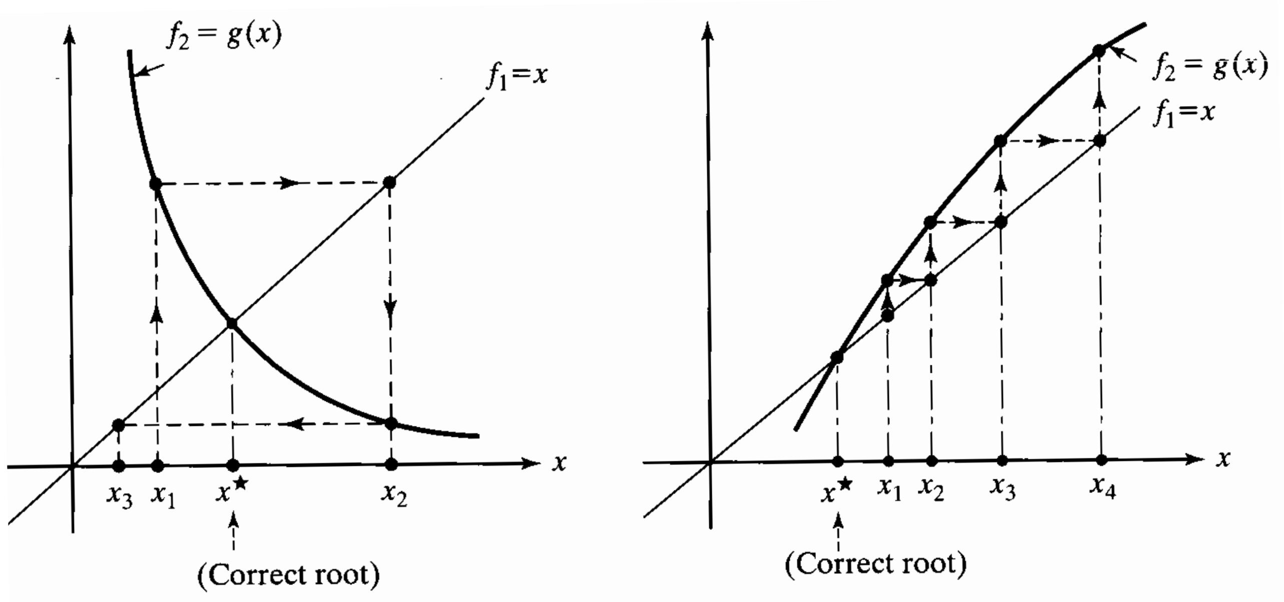


(a) $-1 < g'(x) < 0$; Convergent.

(b) $0 < g'(x) < 1$; Convergent.

Convergence (continue)

- Convergence criterion $|F'(S)| < R < 1$ possesses a simple geometric interpretation



(c) $g'(x) < -1$; Divergent.   (d) $g'(x) > 1$; Divergent.

- What if $F'(S) = 1$? Based on $e_{n+1} \approx e_n F'(S)$, the error will remain constant

Error Estimate

- Based on $e_{n+1} \approx e_n F'(S)$, $x_{n+1} - S \approx (x_n - S)F'(S)$
- It can be shown that $x_{n+1} \approx (x_n - S)\{F'(S) - 1\} + x_n$
- Finally, $x_n - S = e_n \approx \dfrac{x_{n+1} - x_n}{F'(x_{n+1}) - 1}$
- Note that $F'(S)$ can not be evaluated until solution is known. But it can be approximated by $F'(x_{n+1})$
- Iterations are performed when $\left|\dfrac{x_{n+1} - x_n}{F'(x_{n+1}) - 1}\right| < \varepsilon \left|x_{n+1}\right|$

Some Features

- The method is very simple; however, it may not always converge with an arbitrarily chosen form of the function $F(x)$
- The condition to be satisfied for convergence to the correct root is given by $|F'(S)| < 1$
- The convergence of the process is oscillatory if $-1 < F'(x) < 0$, and asymptotic if $0 < F'(x) < 1$. The divergent of the process can occur if $|F'(S)| > 1$

Example of Fixed Point Iteration Method

- The function $f(x) = e^x - 3x^2 = 0$ has 3 roots near 0, 1 and 4. Use the fixed point iteration method to find the 3 roots to 5 significant figures.
- Solution:

$$x = \sqrt{\frac{e^x}{3}}$$

g(x)=sqrt(exp(x)/3)	
i	x
1	1.000000
2	0.9518897
3	0.9292650
4	0.9188121
5	0.9140225
6	0.9118362
7	0.9108400
8	0.9103864
9	0.9101800
10	0.9100860
11	0.9100433
12	0.9100238
13	0.9100150
14	0.9100109

$$x = -\sqrt{\frac{e^x}{3}}$$

g(x)=-sqrt(exp(x)/3)	
i	x
1	0.000000
2	-0.5773503
3	-0.4325829
4	-0.4650559
5	-0.4575660
6	-0.4592828
7	-0.4588887
8	-0.4589791
9	-0.4589584
10	-0.4589632
11	-0.4589621

Example of Fixed Point Iteration Method (continue)

- Solution: Function $f(x) = e^x - 3x^2 = 0$

$$x = \frac{e^x}{3x}$$

g(x)=exp(x)/(3*x)	
i	**x**
1	4.0000000
2	4.5498458
3	6.9319433
4	49.263865
5	1.68025E+19
6	**diverge!**

$$x = \ln\left(3x^2\right)$$

g(x)=ln(3*x^2)	
i	**x**
1	4.0000000
2	3.8712010
3	3.8057419
4	3.7716342
5	3.7536290
6	3.7440585
7	3.7389527
8	3.7362234
9	3.7347629
10	3.7339810
11	3.7335622
12	3.7333379
13	3.7332177
14	3.7331533
15	3.7331188

Newton-Rhapson Method

- A well known and powerful method
- Derived by considering first-order Taylor's series expansion of $f(x)$ about an arbitrary point x_1

$$f(x) \approx f(x_1) + (x - x_1) f'(x_1) = 0$$

- Since the higher order derivative terms were neglected in the approximation of $f(x)$, the solution yields the next approximation to the root as

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

From above, x_2 is an improved approximation to the root

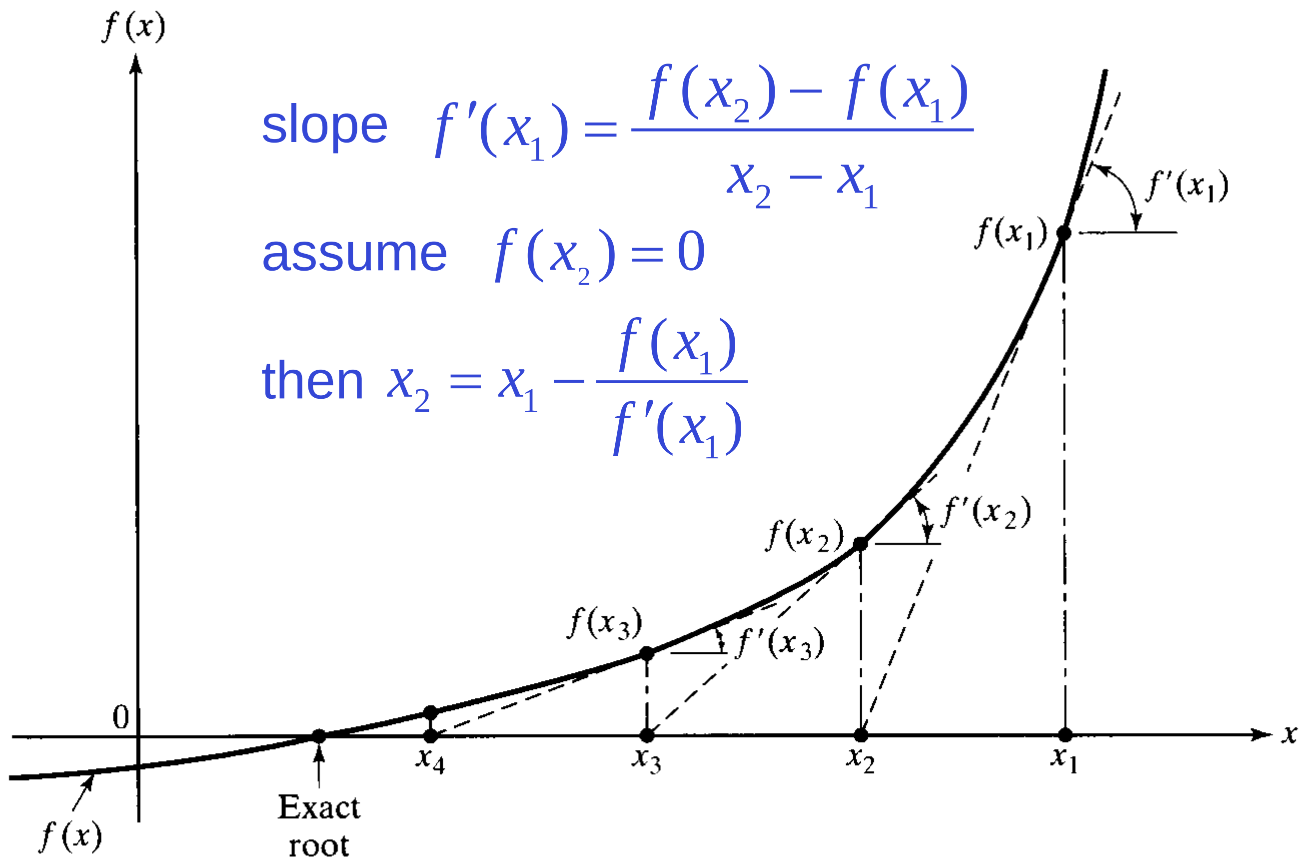
Newton-Rhapson Method (continue)

- Graphically,

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

assume $$f(x_2) = 0$$

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



Newton-Rhapson Method (continue)

- Iterative process can be generalized as

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}, \quad i = 1, 2, 3, \cdots$$

until the approximation x_{i+1} satisfies the ***convergence criterion*** ε,

$$\left| f(x_{i+1}) \right| \le \varepsilon$$

Steps of Solution

- Step 1: Set a value of ε and choose a starting point x_1 and compute $f(x_1)$ and $f'(x_1)$

- Step 2: Calculate $x_2 = x_1 - \dfrac{f(x_1)}{f'(x_1)}$

- Step 3: If $|f(x_2)| \le \varepsilon$, x_2 satisfies the convergence criterion and is the answer. If $|f(x_2)| > \varepsilon$, go to Step 1 with x_2 as the starting value

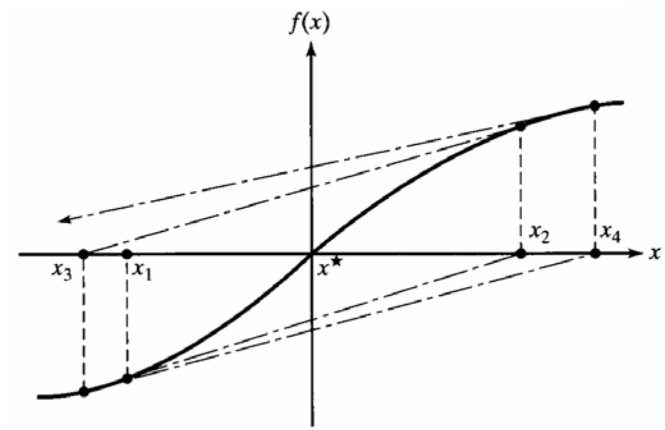
- Repeat Steps 1-3 for $x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x_i)}, i = 3,4,5,\ldots..$ until the procedure satisfies the convergence criterion $|f(x_{i+1})| \le \varepsilon$

Some Features

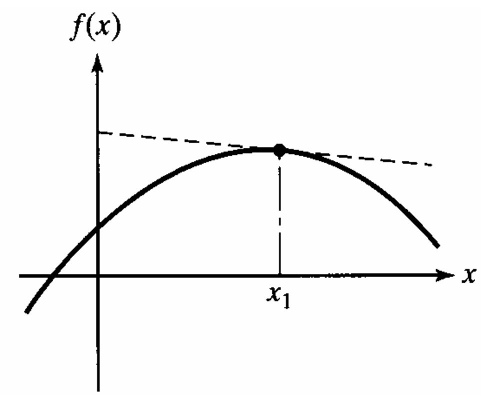
- The Newton's method requires the continuous function $f(x)$ and continuous derivatives $f'(x)$
- The Newton's method is most powerful if $f'(x)$ can be evaluated
- The Newton's method can also be used for finding complex roots, using complex number as the initial guess for the root

Some Features (continue)

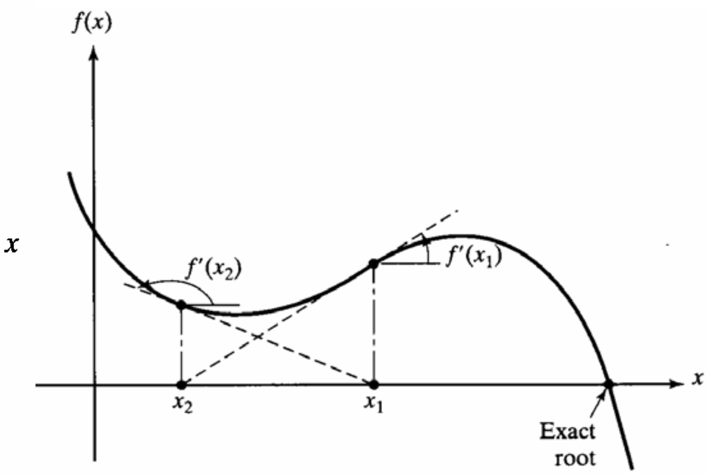
- Newton's method converges very fast in most cases. However it may not converge, if
  - initial guess x_1 is very far from the exact root – (a)
  - $f'(x)$ is close to zero – (b)
  - $f'(x)$ varies substantially near the root – (c)



(a) $f''(x^\star) = 0$ (divergence).



) Derivative (slope) at x_1 close to zero.



(c) Derivative (slope) varies rapidly resulting in oscillation between x_1 and x_2.

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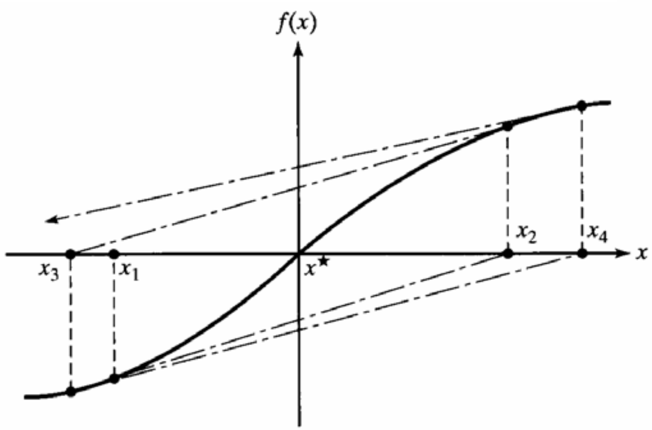

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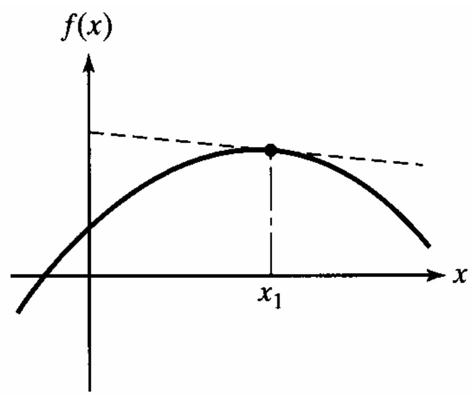

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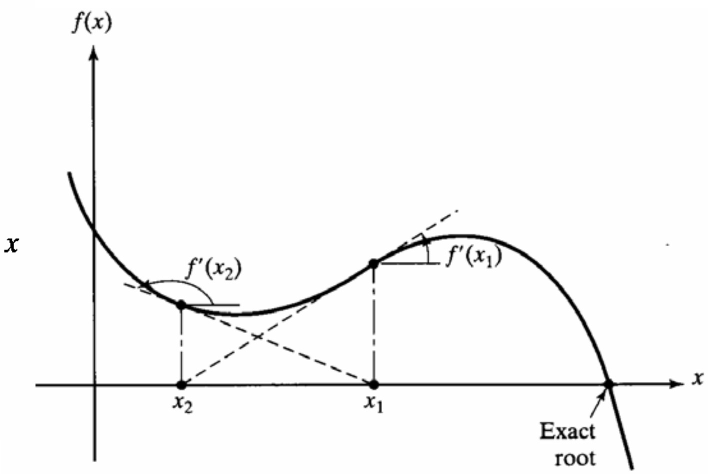
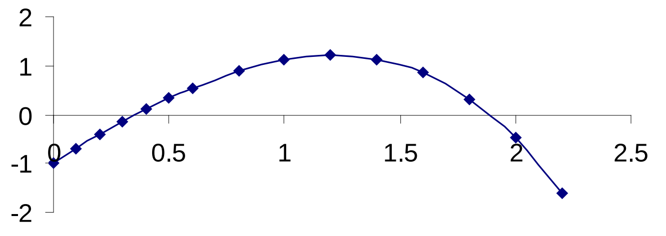


(c) Derivative (slope) varies rapidly resulting in oscillation between x_1 and x_2.

Example of Newton-Rhapson Method

- Use the Newton-Rhapson method to solve $f(x) = 3x + \sin x - e^x$ with a convergence criterion ε =0.001

- Solution:



$$f'(x) = 3 + \cos x - e^x$$

i	x	f(x)	f'(x)
1	0	-1.0000	3.0000
2	0.33333	-0.068426	2.5494
3	0.36017	-6.2977E-04	

i	x	f(x)	f'(x)
1	2	-0.47976	-4.8052
2	1.9002	-0.040396	-4.0107
3	1.8901	-2.7642E-04	-3.9339

i	x	f(x)	f'(x)
1	1	1.1232	0.82202
2	-0.36639	-2.1506	3.2404
3	0.29729	-0.16141	2.6099
4	0.35914	-3.2080E-03	2.5041
5	0.36042	-4.2605E-06	2.5018

i	x	f(x)	f'(x)
1	1.5	1.0158	-1.4110
2	2.2199	-1.7501	-6.8109
3	1.9629	-0.30414	-4.5021
4	1.8953	-2.0835E-02	-3.9734
5	1.8901	-2.7642E-04	-3.9339

Secant Method

- Suppose $f(x)$ is assumed to be linear in the vicinity of the exact root. x_1 and x_2 are assumed to be close to the root. A straight line is drawn through the two points ($f(x_1)$ and $f(x_2)$) and intersect the *x*-axis at x_3. The line through two points on the curve is called the secant line

- If $f(x)$ is truly linear, x_3 would be the root. However, for non-linear function, x_3 should be close to the root

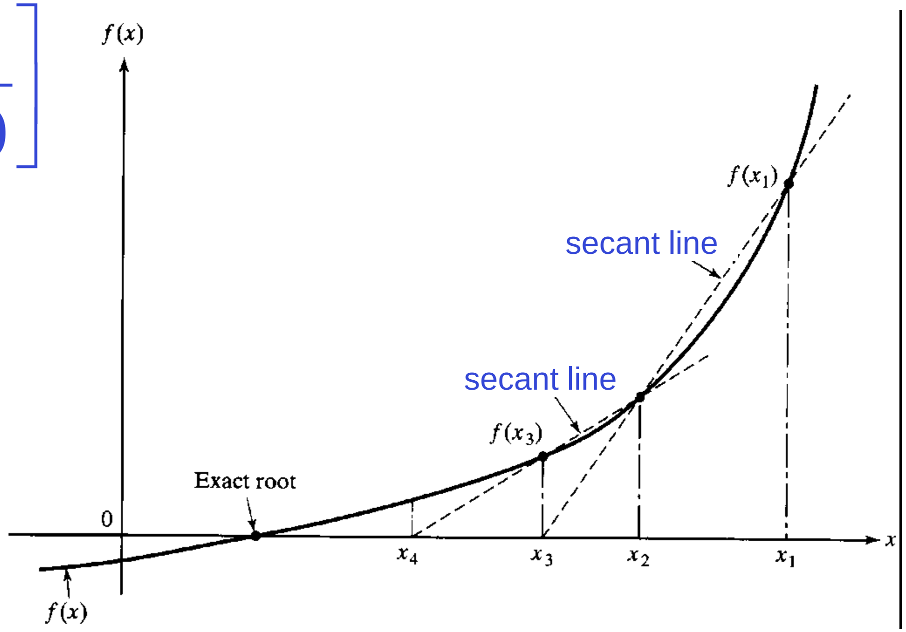
Secant Method (continue)

- Referring to the figure, based on similar two triangles

$$\frac{f(x_2)-f(x_1)}{x_2-x_1}=\frac{0-f(x_2)}{x_3-x_2}$$

- Rewriting in the form to solve x_3

$$x_3 = x_2 - f(x_2)\left[\frac{x_2-x_1}{f(x_2)-f(x_1)}\right]$$



Steps of Solution

- Step 1: Start with two initial approximations x_1 and x_2 and a small value of ε. Calculate $f(x_1)$ and $f(x_2)$

- Step 2: Find the new approximation, x_{n+1} as

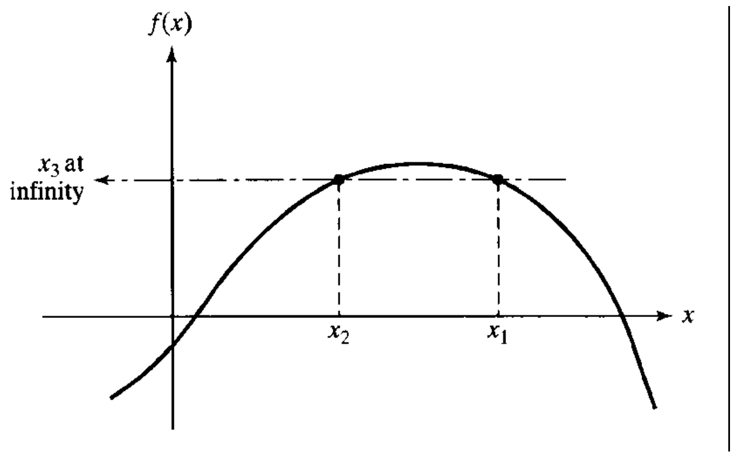
$$x_{i+1} = x_i - \frac{f(x_i)\left(x_i - x_{i-1}\right)}{f(x_i) - f(x_{i-1})} \quad i = 2, 3, 4, \ldots$$

- Verify the convergence. If $\left| f(x_{i+1}) \right| \leq \varepsilon$, halt the process by taking x_{i+1} as a root. Otherwise, update the iteration number as $i = i + 1$ and go to Step 2

Some Features

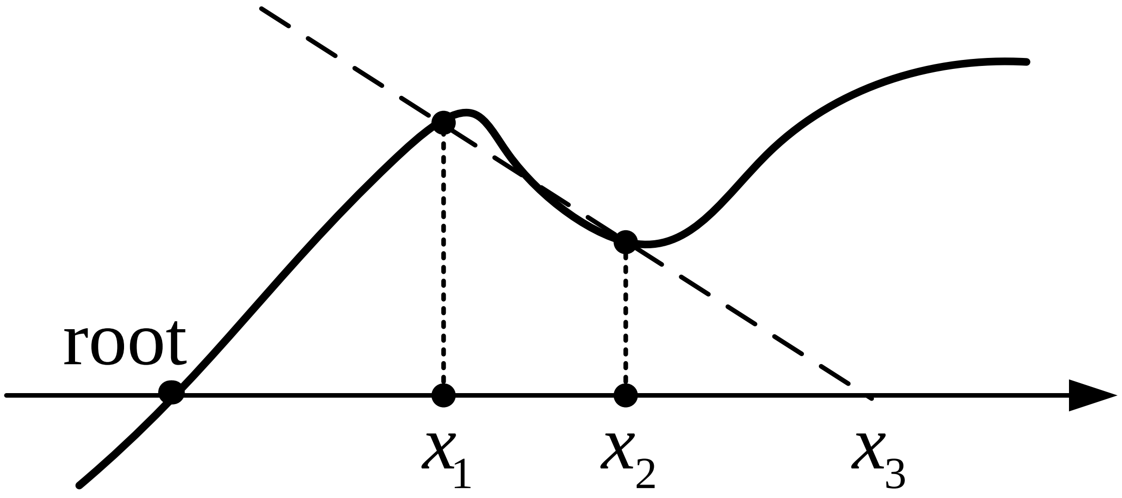
- The Secant method is preferred over the Newton-Raphson method, when the evaluation of $f'(x)$ is difficult
- Since $f'(x_i) \approx \left[\dfrac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \right]$, the process may not

  converge if $f(x_1) \approx f(x_2)$ in which the next approximation (x_3) will be near infinity (see Figure below)



Some Features (continue)

- If the function is far from linear near the root, the successive iterates can fly off to points far from the root, as seen in Figure below



Example of Secant Method

- Use the Secant method to solve $x^3 + x^2 - 3x = 3$ with (x_1, x_2) = (1,2) and a convergence criterion ε =10^{-5}

- Solution:

$f(x_1)$ $f(x_2)$

i	x	f(x)	|f(x)| < ε ?
1	1	-4	no
2	2	3	no
3	1.571429	-1.364428	no
4	1.705411	-0.2477435	no
5	1.735136	2.929758E-02	no
6	1.731993	-5.470760E-04	no
7	1.732051	1.821188E-06	yes

Systems of Nonlinear Equations

- The problem of finding the solution of a set of nonlinear equations can be solved using Newton-Rhapson Method
- Take for example,

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

Applying Taylor series expansions about point (x_i, y_i) for point (x_{i+1}, y_{i+1})

$$f_1(x_{i+1}, y_{i+1}) = f_1(x_i, y_i) + (x_{i+1} - x_i)\frac{\partial f_1(x_i, y_i)}{\partial x} + (y_{i+1} - y_i)\frac{\partial f_1(x_i, y_i)}{\partial y} = 0$$

$$f_2(x_{i+1}, y_{i+1}) = f_2(x_i, y_i) + (x_{i+1} - x_i)\frac{\partial f_2(x_i, y_i)}{\partial x} + (y_{i+1} - y_i)\frac{\partial f_2(x_i, y_i)}{\partial y} = 0$$

Systems of Nonlinear Equations (continue)

- Truncating the series gives

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{Bmatrix} f_1(x_i, y_i) \\ f_2(x_i, y_i) \end{Bmatrix} + \begin{bmatrix} \dfrac{\partial f_1(x_i, y_i)}{\partial x} & \dfrac{\partial f_1(x_i, y_i)}{\partial y} \\ \dfrac{\partial f_2(x_i, y_i)}{\partial x} & \dfrac{\partial f_2(x_i, y_i)}{\partial y} \end{bmatrix} \begin{Bmatrix} x_{i+1} - x_i \\ y_{i+1} - y_i \end{Bmatrix}$$

- Rewrite this to solve as the system of equations

$$\begin{bmatrix} \dfrac{\partial f_1(x_i, y_i)}{\partial x} & \dfrac{\partial f_1(x_i, y_i)}{\partial y} \\ \dfrac{\partial f_2(x_i, y_i)}{\partial x} & \dfrac{\partial f_2(x_i, y_i)}{\partial y} \end{bmatrix} \begin{Bmatrix} \Delta x_i \\ \Delta y_i \end{Bmatrix} = \begin{Bmatrix} -f_1(x_i, y_i) \\ -f_2(x_i, y_i) \end{Bmatrix} \quad \text{where} \quad \begin{Bmatrix} \Delta x_i \\ \Delta y_i \end{Bmatrix} = \begin{Bmatrix} x_{i+1} - x_i \\ y_{i+1} - y_i \end{Bmatrix}$$

Systems of Nonlinear Equations (continue)

- Solve for $\begin{Bmatrix} \Delta x_i \\ \Delta y_i \end{Bmatrix}$ by Gaussian elimination and then improve the an estimate of the root $\begin{Bmatrix} x_{i+1} \\ y_{i+1} \end{Bmatrix}$ as $\begin{matrix} x_{i+1} = x_i + \Delta x_i \\ y_{i+1} = y_i + \Delta y_i \end{matrix}$
- Repeat this process with i replaced by i + 1 until $f_1(x, y)$ and $f_2(x, y)$ are close to 0
- It is interesting to observe that Newton's method, as applied to a set of nonlinear equations, reduces the problem to solving a set of linear equations in order to determine the values that improve the accuracy of the estimates