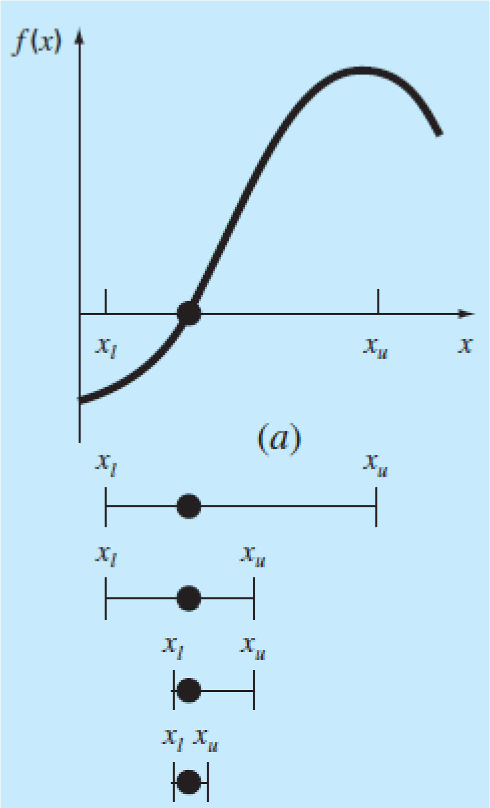
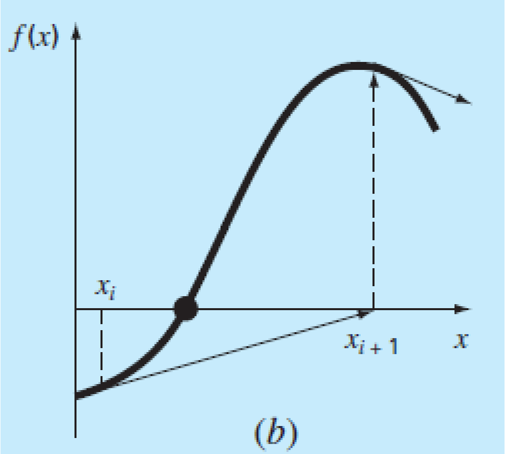
Open Methods

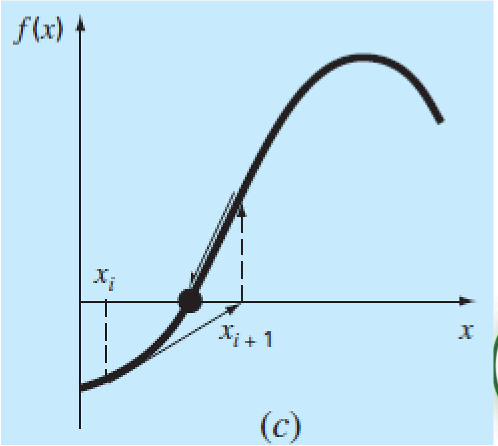
Chapra: Chapter-6

Open Methods

- Bracketing method results in closer estimates of the true value of root. This method is said to be convergent.
- Open method requires single value of *x* or two values that do not necessarily bracket the true root. Rather they may move away from the root but when they converge, they do much more quickly.







Roots of Equations

- Roots of Equations
  - Bracketing Methods
    - Bisection method
    - False Position Method
  - Open Methods
    - Simple fixed point iteration
    - Newton Raphson
    - Secant
    - Modified Newton Raphson
  - System of Nonlinear Equations
  - Roots of polynomials
    - Muller Method

Simple Fixed-Point Iteration

- It is also called one-point iteration or successive substitution.
- The function $f(x) = 0$ is rearranged so that x can be on the left-hand side of the equation. For example:

$$x^2 - 2x + 3 = 0$$

$$x = \frac{x^2 + 3}{2}$$

- The purpose is to predict a new value of x as a function of an old value of x. The formula can be $x_{i+1} = g(x_i)$
- Approximate error of this equation is $\varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \times 100\%$

Simple Fixed-Point Iteration

- Use simple fixed-point iteration to locate the root of $f(x) = e^{-x} - x$
- The function can be rearranged in the form $x_{i+1} = e^{-x_i}$

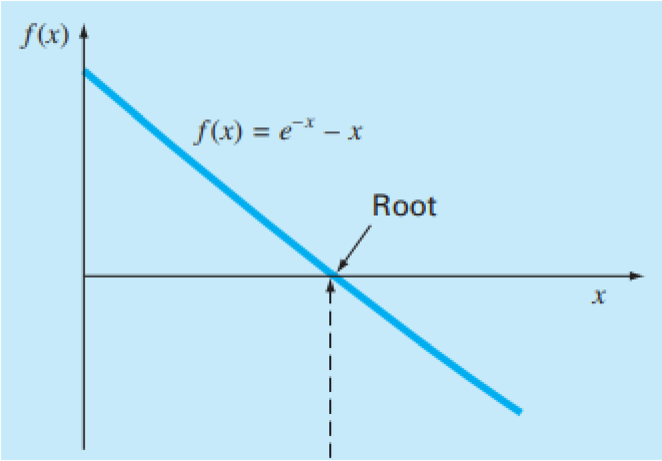
Iter.	x_i	$e_a\%$	$e_t\%$
1	0		100.0
2	1.00	100.0	76.3
3	0.367	171.8	35.1
4	0.692	46.9	22.1
5	0.500	38.3	11.8
6	0.606	17.4	6.89
7	0.545	11.2	3.83
8	0.579	5.90	2.20
9	0.560	3.48	1.24
10	0.571	1.93	0.70

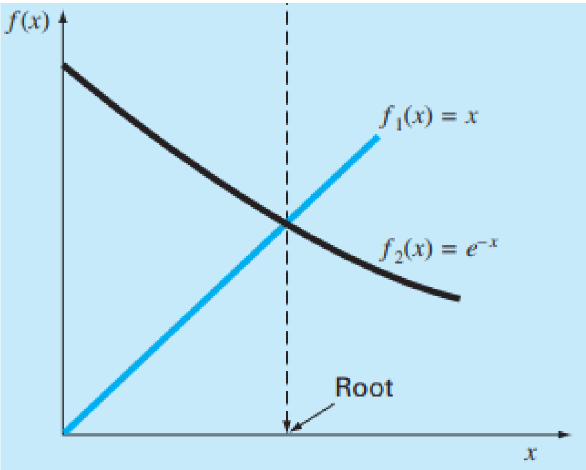
True root is 0.567

Two-Curve Graphical Method

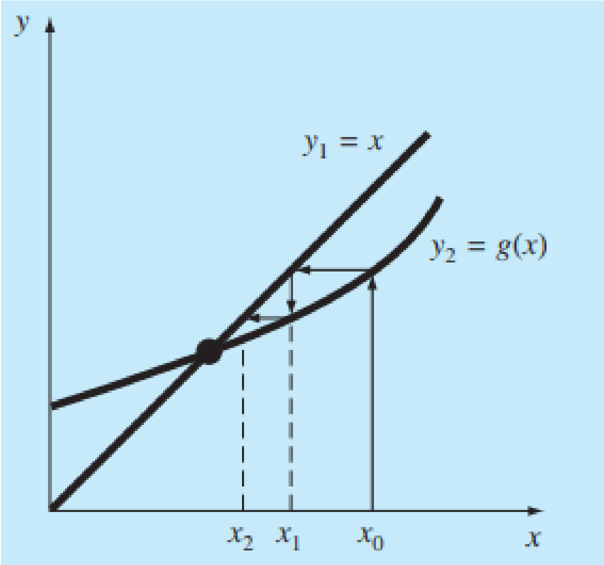
- Separate the equation $e^{-x} - x = 0$ into two parts and determine its root graphically.
- Reformulate the equation as $y_1 = x$ and $y_2 = e^{-x}$. The following values can be computed

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

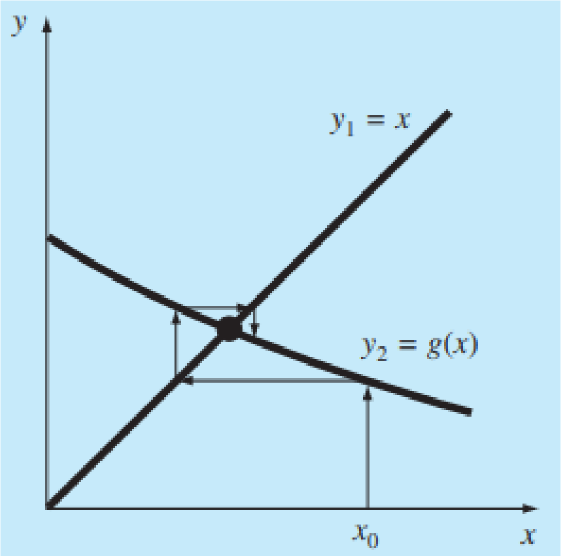




Convergence Example

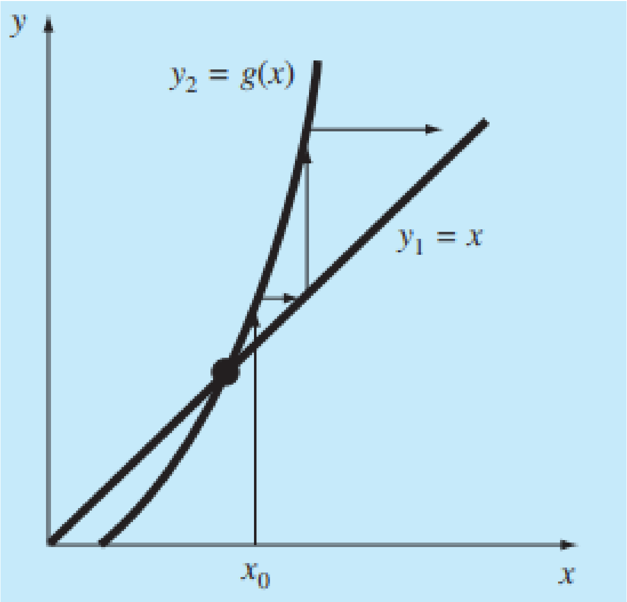


Convergent staircase pattern

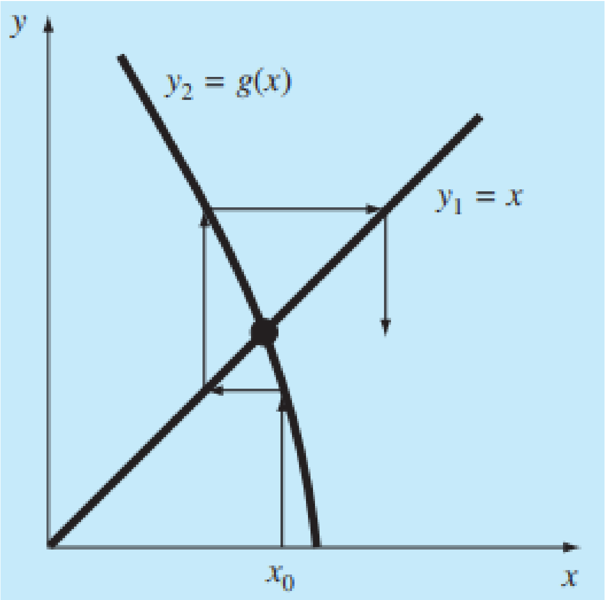


Convergent spiral pattern

Divergence Example



Divergent staircase pattern



Divergent spiral pattern

Convergence?

If $x = a$ is a solution then,

$$
\begin{aligned}
x_{n+1} &= g(x_n) \\
&= g(a+\varepsilon_n) \\
&= g(a) + \varepsilon_n g'(a) + \tfrac{1}{2}\varepsilon_n^2 g''(a) + \cdots \\
&\approx a + \varepsilon_n g'(a) \qquad [\varepsilon_n \approx 0 \text{ and } g(a) = a]
\end{aligned}
$$

$$\boxed{f(x) \approx f(a) + \sum_{i \le n} \frac{f^{(i)}(a)}{i!}(x-a)^i}$$

$$\varepsilon_{n+1} \approx \varepsilon_n g'(a) \qquad [\varepsilon_{n+1} = x_{n+1} - a]$$

$$\boxed{\therefore\ \varepsilon_{n+1} < \varepsilon_n} \qquad \boxed{\text{if } |g'(a)| < 1}$$

error reduces at each step
i.e. iteration will converge

If magnitude of 1st derivative at x=a is less than 1

Problem

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

- Find a root near *x=1.0* and *x=2.0*
- Solution:

$$x = g(x) = \tfrac{1}{2}x^2 + \tfrac{1}{4}$$

  - Starting at x=1, x=0.292893 at 15th iteration
  - Starting at x=2, it will not converge
  - Why? Relate to *g'(x)=x*. for convergence *g'(x) < 1*

$$x = g(x) = \sqrt{2x - \tfrac{1}{2}}$$

  - Starting at x=1, x=1.707 at iteration 19
  - Starting at x=2, x=1.707 at iteration 12
  - Why? Relate to

$$g'(x) = \left(2x - \tfrac{1}{2}\right)^{-\tfrac{1}{2}}$$

Newton Raphson Method

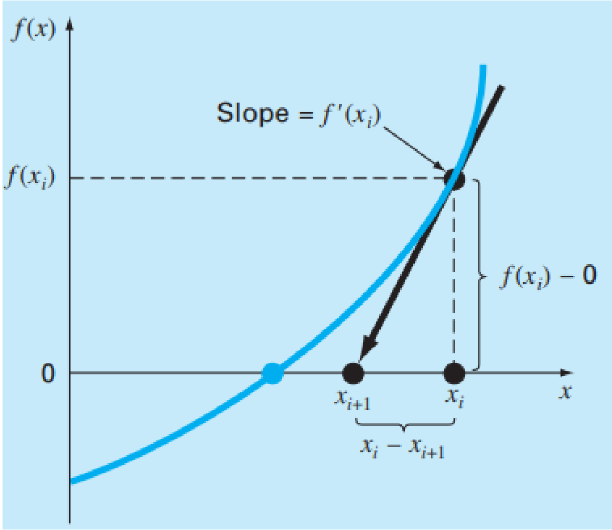
- Most widely used of all root-locating formulae.
- For an initial guess x_i, a tangent can be extended from the point $[x_i, f(x_i)]$.
- The point where the tangent crosses the x axis usually represents an improved estimate of the root.

$$x_i = \text{approximate root}$$

$$x_{i+1} = \text{intersection of } f'(x_i) \text{ and } x\text{-axis}$$

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

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



Newton Raphson Method

- Use the Newton-Raphson method to estimate the root of $f(x) = e^{-x} - x$, employing an initial guess of $x_0 = 0$
- The first derivative of the function can be evaluated as

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

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

The true percent relative error at each iteration decreases much faster than it does in simple fixed-point iteration.

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	$< 10^{-8}$

Convergence

Taylor series expansion is

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

For approximate solution:

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

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

$f(x_{i+1}) = 0$ at intersection with x – axis

For exact solution:

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

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

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

$$\boxed{E_{t,i+1} = \frac{-f''(x_r)}{2f'(x_r)} E_{t,i}^2}$$

Example

- The error is roughly proportional to the square of the previous error, as in

$$E_{t,i+1} = \frac{-f''(x_r)}{2f'(x_r)} E_{t,i}^2$$

Examine this formula and see if it applies to the results of previous example.

- The first derivative of $f(x) = e^{-x} - x$ is $f'(x) = -e^{-x} - 1$

which can be evaluated at $x_r = 0.56714329$ as

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

The second derivative is $f''(x) = e^{-x}$

$$f''(0.56714329) = 0.56714329$$

Example

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

In the previous example, the initial error was $E_{t,0} = 0.56714329$

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

$$E_{t,2} \cong 0.18095(0.06714329)^2 = 0.0008158$$

$$E_{t,3} \cong 0.18095(0.0008323)^2 = 0.000000125$$

$$E_{t,4} \cong 0.18095(0.000000125)^2 = 2.83 \times 10^{-15}$$

x_i	E_t
0	0.56714329
0.500000000	0.06714329
0.566311003	0.00083228
0.567143165	0.000000125

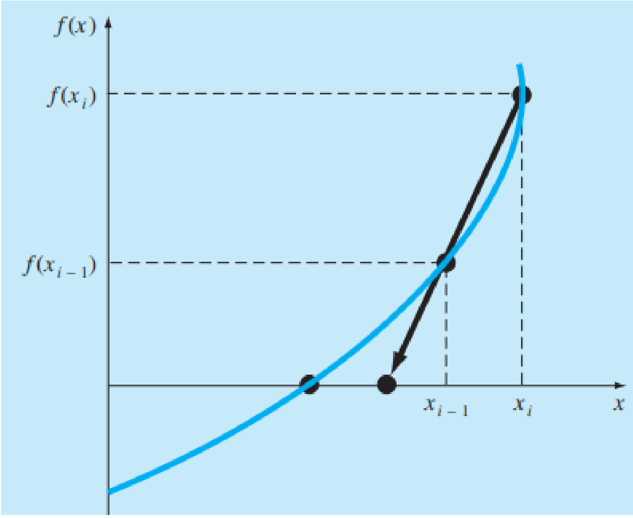
The error of the Newton-Raphson method for this case is, in fact, roughly proportional (by a factor of 0.18095) to the square of the error of the previous iteration.

Secant Method

- Newton-Raphson method needs to compute $f'(x)$
  - It may be analytically complicated, or
  - Numerical evaluation may be time consuming
- the derivative can be approximated by a backward finite divided difference

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

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



This approach requires two initial estimates of *x*.

Secant Method

- Use the secant method to estimate the root of $f(x) = e^{-x} – x$. Start with initial estimates of $x_{-1} = 0$ and $x_0 = 1.0$.
- The true root is 0.56714329..
- First iteration: $x_{-1} = 0$ and $x_0 = 1.0$

  $f(x_{-1}) = 1.00000$ and $f(x_0) = – 0.63212$

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

- Second iteration: $x_0 = 1$ and $x_1 = 0.61270$

  $f(x_0) = – 0.63212$ and $f(x_1) = – 0.07081$

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

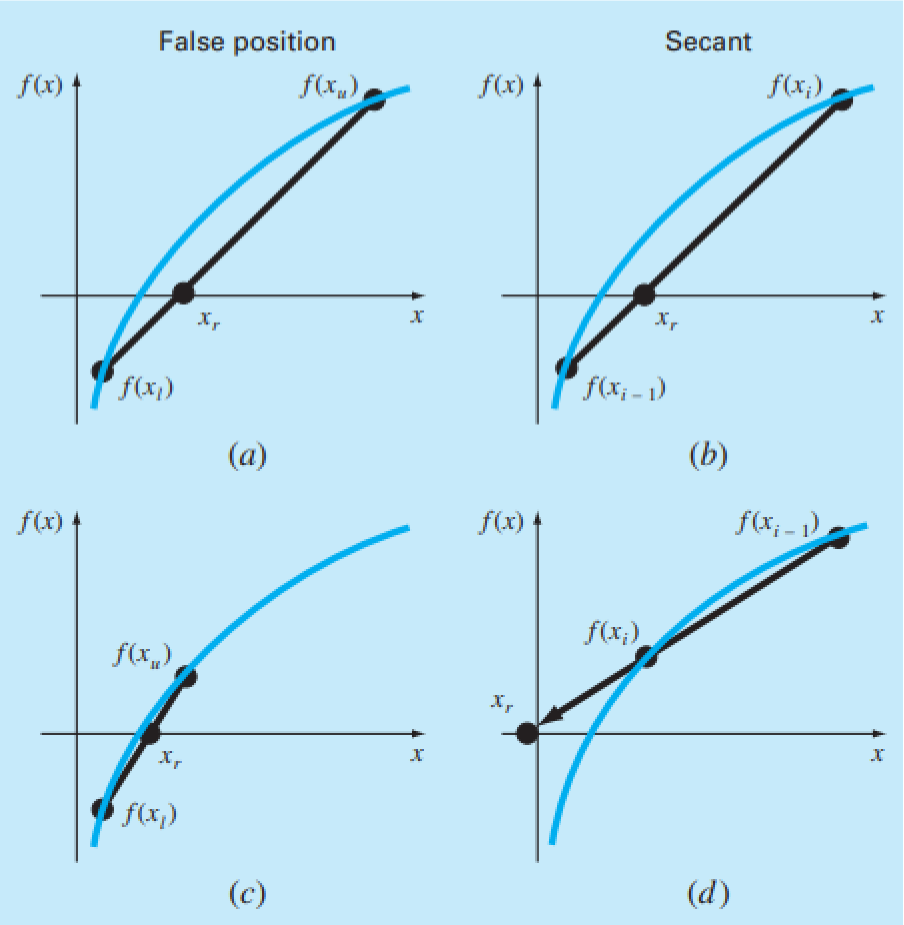
Secant Method

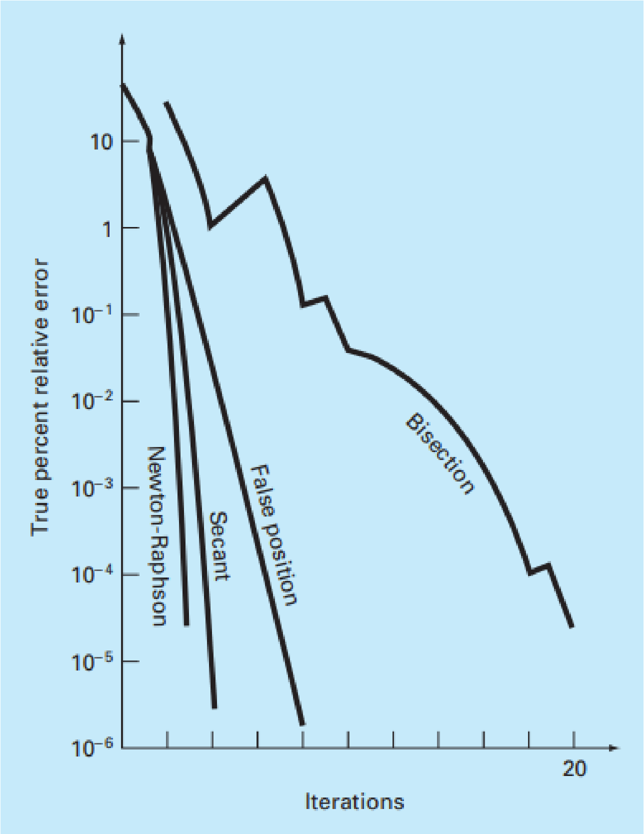
- Third iteration: $x_1 = 0.61270$ and $x_2 = 0.56384$

  $f(x_1) = – 0.07081$ and $f(x_2) = 0.00518$

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

Difference between Secant and False-Position Methods





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 $f'(x)$

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

where δ = a small perturbation fraction.

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

Example

- Use the modified secant method to estimate the root of $f(x) = e^{-x} - x$. Use a value of 0.01 for δ and start with $x_0 = 1.0$. Recall that the true root is 0.56714329. . . .
- First iteration:

$$x_0 = 1 \qquad f(x_0) = -0.63212$$
$$x_0 + \delta x_0 = 1.01 \qquad f(x_0 + \delta x_0) = -0.64578$$
$$x_1 = 1 - \frac{0.01(-0.63212)}{-0.64578 - (-0.63212)} = 0.537263 \qquad |\varepsilon_t| = 5.3\%$$

- Second iteration:

$$x_0 = 0.537263 \qquad f(x_0) = 0.047083$$
$$x_0 + \delta x_0 = 0.542635 \qquad f(x_0 + \delta x_0) = 0.038579$$
$$x_1 = 0.537263 - \frac{0.005373(0.047083)}{0.038579 - 0.047083} = 0.56701 \qquad |\varepsilon_t| = 0.0236\%$$

Example

- Third iteration:

$$x_0 = 0.56701 \qquad f(x_0) = 0.000209$$

$$x_0 + \delta x_0 = 0.572680 \qquad f(x_0 + \delta x_0) = -0.00867$$

$$x_1 = 0.56701 - \frac{0.00567(0.000209)}{-0.00867 - 0.000209} = 0.567143 \qquad |\varepsilon_t| = 2.365 \times 10^{-5}\%$$

- 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.
- If it is too big, the technique can become inefficient and even divergent.