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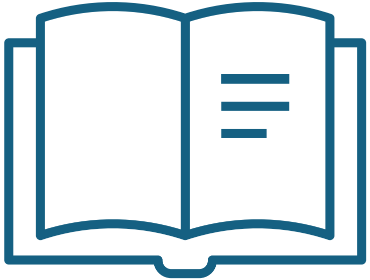
DEPARTMENT OF CIVIL AND ENVIRONMENTAL ENGINEERING
BACHELOR IN CIVIL ENGINEERING

Numerical Methods

Roots of Equations

Roots of equations



- Reference
  - Chapra, S.C., Canale, R.P., 2015, *Numerical Methods for Engineers*, 7th Ed., McGraw-Hill Book Co., New York
    - Part Two: Chapters 5 to 8 (pp 117 to 229)

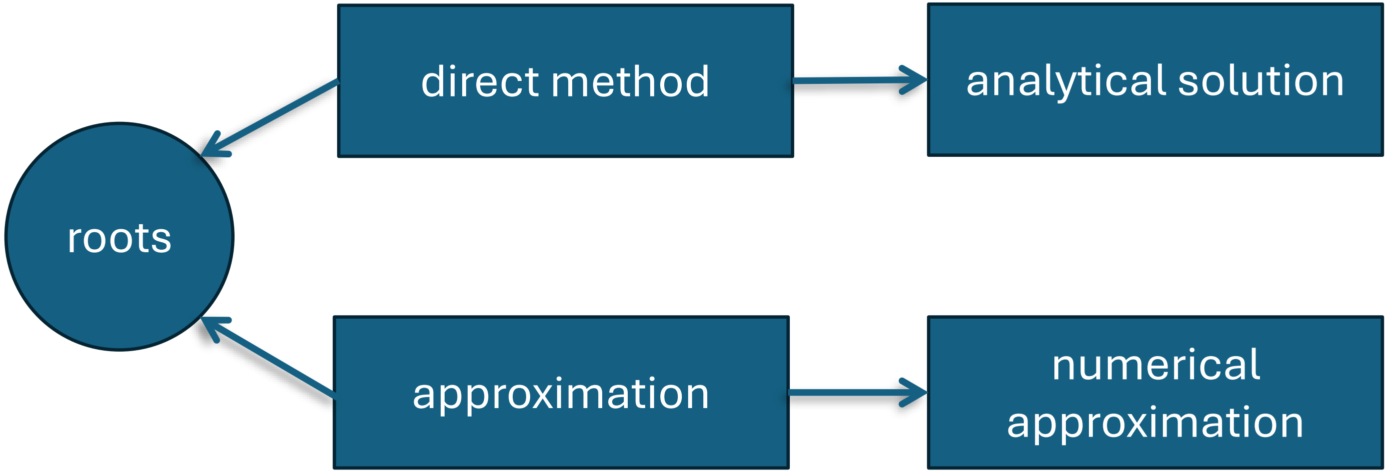
Roots of equations

$$y = f(x) = ax^2 + bx + c = 0$$ a quadratic formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$ solution of the quadratic formula

- The values obtained from the solution of the quadratic formula are called the "roots" of the formula
- The roots represent the values of x that make the $f(x)$ equal to zero
- Definition
  - the root of an equation is the value of x that makes $f(x) = 0$
  - roots are sometimes called the zeros of the equation
- The root of a quadratic formula is easy to solved, but
  - there are many equations for which the root cannot be easily determined

How to solve for roots of equations



Methods to solve for roots of equations

Bracketing methods

- Graphical methods
- The bisection method
- The false-position method

Open methods

- Simple fixed-point iteration
- The Newton-Raphson method
- The secant method
- Multiple roots

Graphical methods

Fall velocity of a parachutist

gravitational acceleration

mass of the parachutist

time

$$v = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right)$$

fall velocity

drag coefficient

Problem statement
Find c when $v = 40$ m/s, $m = 68.1$ kg, $t = 10$ s, $g = 9.8$ m/s^2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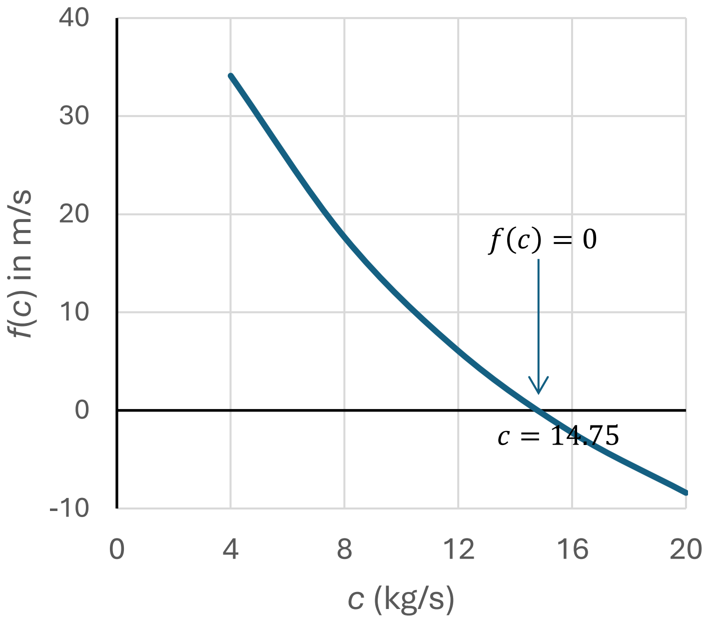
Graphical methods

$$v = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right) \implies 40 = \frac{9.8(68.1)}{c}\left(1 - e^{-(c/68.1)10}\right)$$

$$\iff \underbrace{\frac{9.8(68.1)}{c}\left(1 - e^{-(c/68.1)10}\right) - 40 = 0}_{f(c) = 0}$$

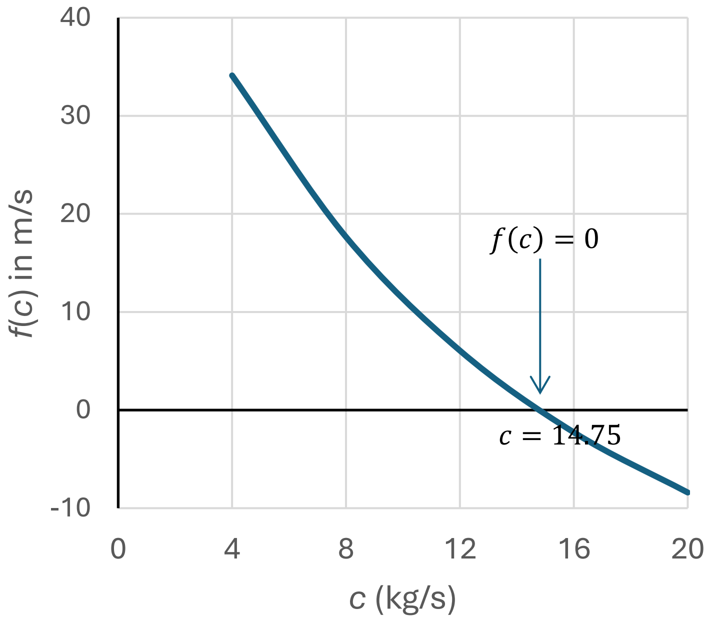


c (kg/s)	$f(c)$ in m/s
4	34.1148
8	17.6534
12	6.0669
16	−2.2688
20	−8.4006

Note that c is in kg/s and $f(c)$ is in m/s

Graphical methods

$$v = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right) \quad \Longrightarrow 40 = \frac{9.8(68.1)}{c}\left(1 - e^{-(c/68.1)10}\right)$$



$$\Longleftrightarrow \underbrace{\frac{9.8(68.1)}{c}\left(1 - e^{-(c/68.1)10}\right) - 40 = 0}_{f(c) = 0}$$

$$f(14.75) = \frac{9.8(68.1)}{14.75}\left(1 - e^{-(14.75/68.1)10}\right) - 40 = 0.059$$

$$v = \frac{9.8(68.1)}{14.75}\left(1 - e^{-(14.75/68.1)10}\right) = 40.059 \text{ m/s}$$

Estimate of error $\epsilon_a = \left|\frac{c^{new} - c^{old}}{c^{new}}\right| 100\%$

Graphical methods

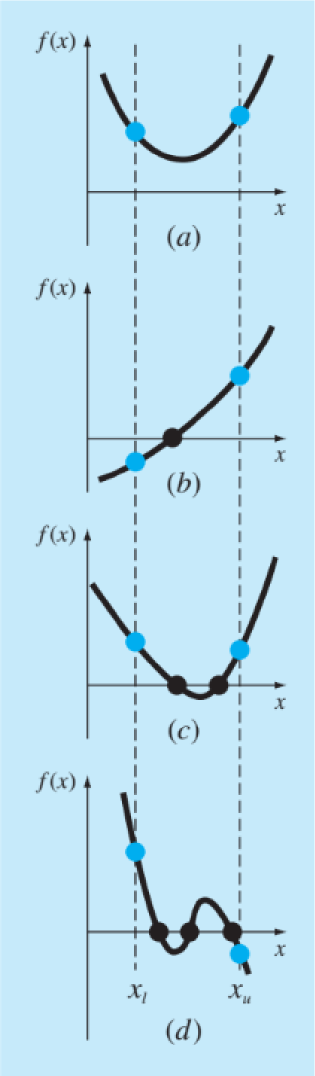
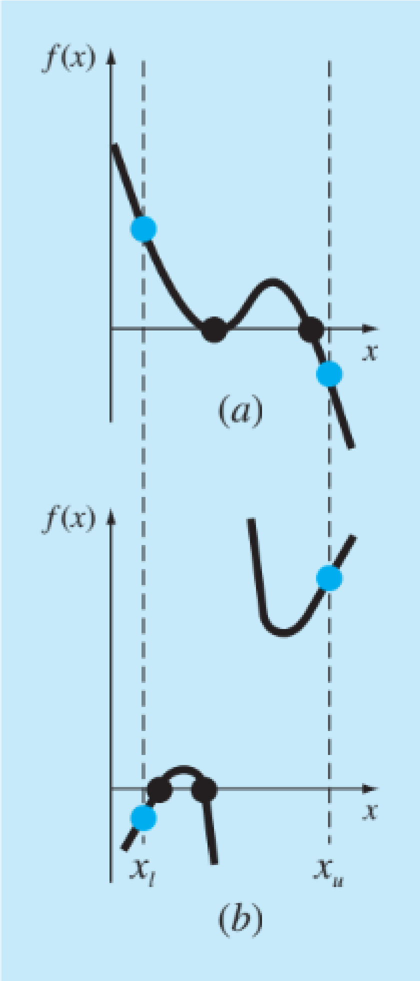


FIGURE 5.2
Illustration of a number of general ways that a root may occur in an interval prescribed by a lower bound x_l and an upper bound x_u. Parts (*a*) and (*c*) indicate that if both $f(x_l)$ and $f(x_u)$ have the same sign, either there will be no roots or there will be an even number of roots within the interval. Parts (*b*) and (*d*) indicate that if the function has different signs at the end points, there will be an odd number of roots in the interval.

Graphical methods

FIGURE 5.3

Illustration of some exceptions to the general cases depicted in Fig. 5.2. (*a*) Multiple root that occurs when the function is tangential to the *x* axis. For this case, although the end points are of opposite signs, there are an even number of axis intersections for the interval. (*b*) Discontinuous function where end points of opposite sign bracket an even number of roots. Special strategies are required for determining the roots for these cases.



Graphical methods

Problem Statement. Computer graphics can expedite and improve your efforts to locate roots of equations. The function

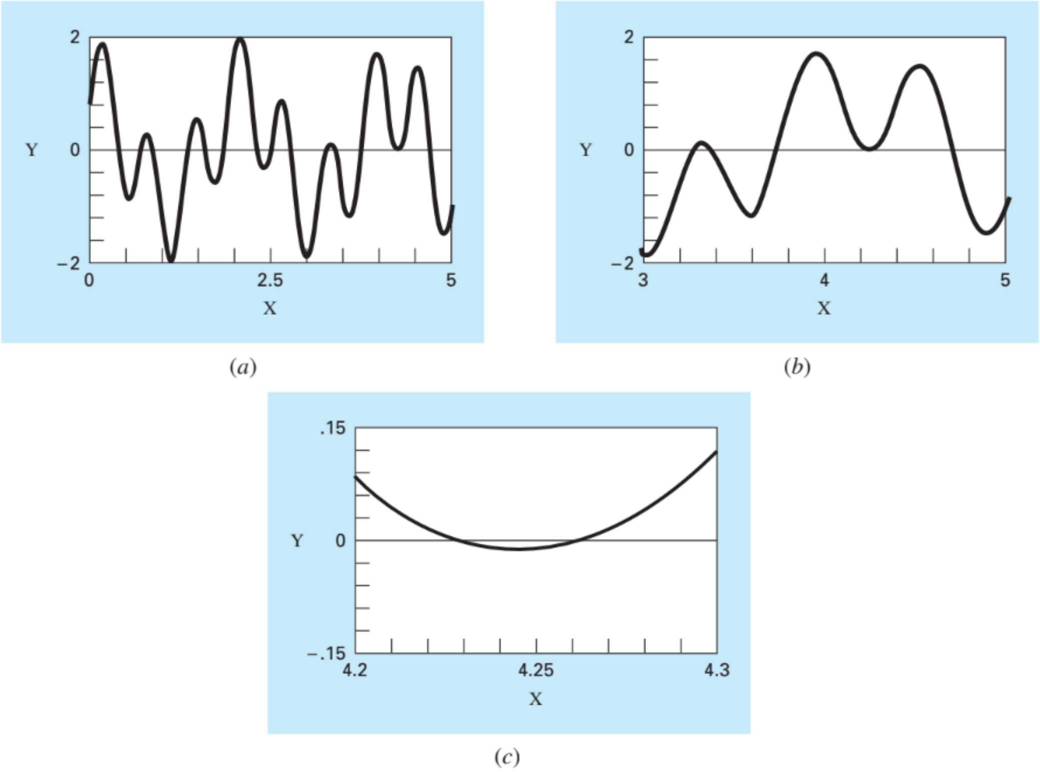
$$f(x) = \sin 10x + \cos 3x$$

has several roots over the range $x = 0$ to $x = 5$. Use computer graphics to gain insight into the behavior of this function.

- use an application
- write a computer program

Graphical methods

FIGURE 5.4
The progressive enlargement of $f(x) = \sin 10x + \cos 3x$ by the computer. Such interactive graphics permits the analyst to determine that two distinct roots exist between $x = 4.2$ and $x = 4.3$.



The bisection method

$f(x) = 0$

- Steps
  1. Choose lower x_l and upper x_u guesses for the root suct that the function changes sign over the interval
  2. An estimate of the root x_r is determined by

$$x_r = \frac{x_l + x_u}{2}$$

  3. Make the following evaluations to determine in which subinterval the root lies
     a) if $f(x_l)f(x_r) < 0$, the root lies in the lower subinterval; therefore, set $x_u = x_r$ and return to step 2
     b) if $f(x_l)f(x_r) > 0$, the root lies in the upper subinterval; therefore, set $x_l = x_r$ and return to step 2
     c) if $f(x_l)f(x_u) = 0$, the root equals x_r; terminate the computation

The bisection method

$$f(c) = 0$$

$$\Leftrightarrow \frac{9.8(68.1)}{c}\left(1 - e^{-(c/68.1)10}\right) - 40 = 0$$

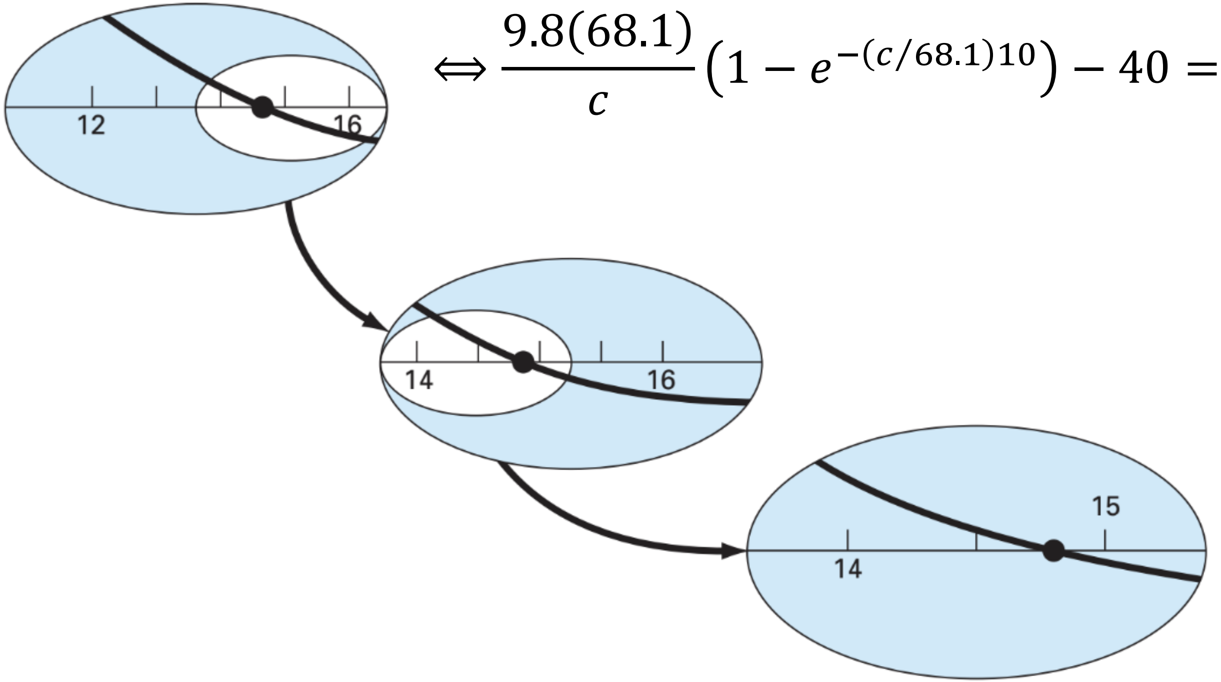


FIGURE 5.6
A graphical depiction of the bisection method. This plot conforms to the first three iterations from Example 5.3.

The bisection method

$$\epsilon_a = \left| \frac{c_r^{new} - c_r^{old}}{c_r^{new}} \right| 100\%$$

i	c_i	$f(c_i)$	c_r	Δc_r	ϵ_a (%)
0	12	6.0669			
1	16	-2.2688	14		
2	14	1.5687	15	1	6.6667
3	15	-0.4248	14.5	1	6.8966
4	14.5	0.5523	14.75	-0.5	3.3898
5	14.75	0.0590	14.875	0.25	1.6807
6	14.875	-0.1841	14.8125	0.125	0.8439
7	14.8125	-0.0629	14.7813	-0.0625	0.4228
8	14.7813	-0.0020	14.7656	-0.0313	0.2116
9	14.7656	0.0284	14.7734	-0.0156	0.1058

The bisection method

- The above calculation table is compact but it may not be easily readable
- The following table is longer than this one, but it is more readable than the above table
  - The c_l and c_u for the iteration number $i > 0$ are

$$f(c_{l,i-1})f(c_{r,i-1}) = \begin{cases} < 0 & \Rightarrow c_{l,i} = c_{l,i-1} \wedge c_{u,i} = c_{r,i-1} \\ > 0 & \Rightarrow c_{l,i} = c_{r,i-1} \wedge c_{u,i} = c_{u,i-1} \end{cases}$$

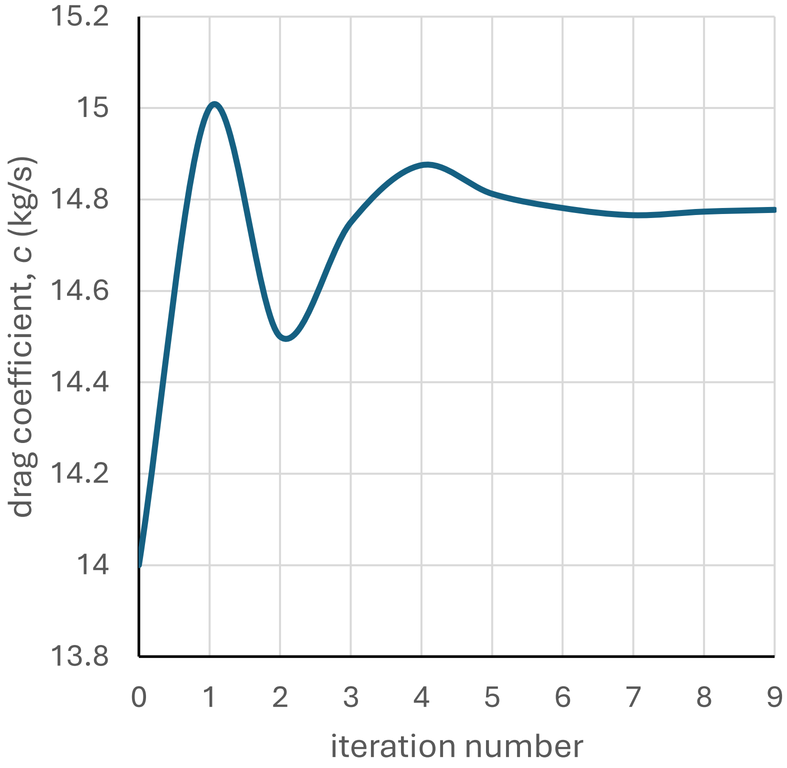
- Please note that c is in kg/s unit and $f(c)$ is in m/s unit

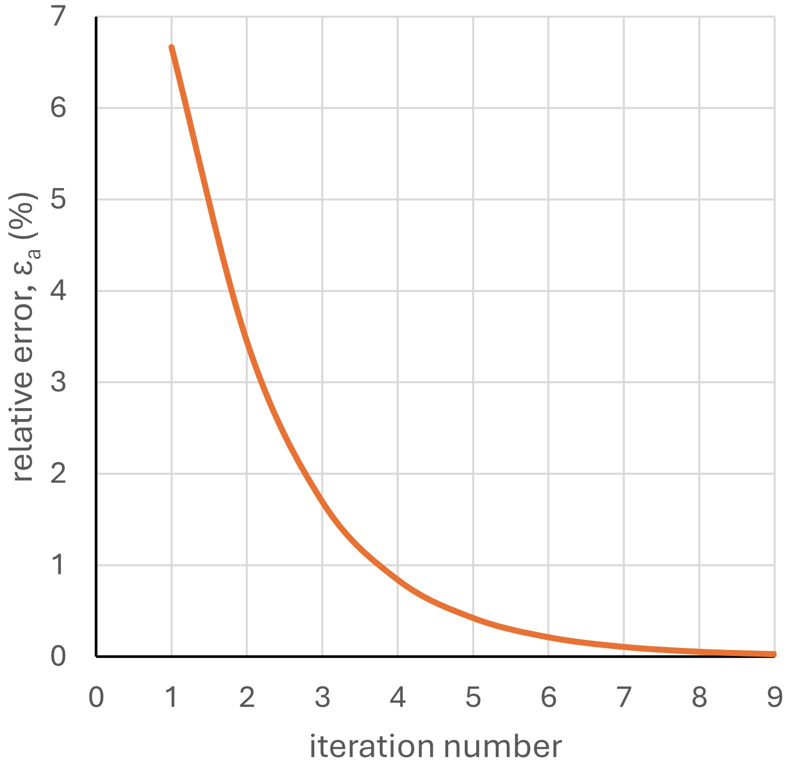
The bisection method

$$\epsilon_a = \left| \frac{c_r^{new} - c_r^{old}}{c_r^{new}} \right| 100\%$$

i	c_l	$f(c_l)$	c_u	$f(c_u)$	c_r	$f(c_r)$	$f(c_l)f(c_r)$	ϵ_a (%)
0	12	6.0669	16	-2.2688	14	1.5687	9.5172	
1	14	1.5687	16	-2.2688	15	-0.4248	-0.6664	6.6667
2	14	1.5687	15	-0.4248	14.5	0.5523	0.8664	3.4483
3	14.5	0.5523	15	-0.4248	14.75	0.0590	0.0326	1.6949
4	14.75	0.0590	15	-0.4248	14.875	-0.1841	-0.0109	0.8403
5	14.75	0.0590	14.8750	-0.1841	14.8125	-0.0629	-0.0037	0.4219
6	14.75	0.0590	14.8125	-0.0629	14.7813	-0.0020	-0.0001	0.2114
7	14.75	0.0590	14.7813	-0.0020	14.7656	0.0284	0.0017	0.1058
8	14.7656	0.0284	14.7813	-0.0020	14.7734	0.0132	0.0004	0.0529
9	14.7734	0.0132	14.7813	-0.0020	14.7773	0.0056	0.0001	0.0264

The bisection method

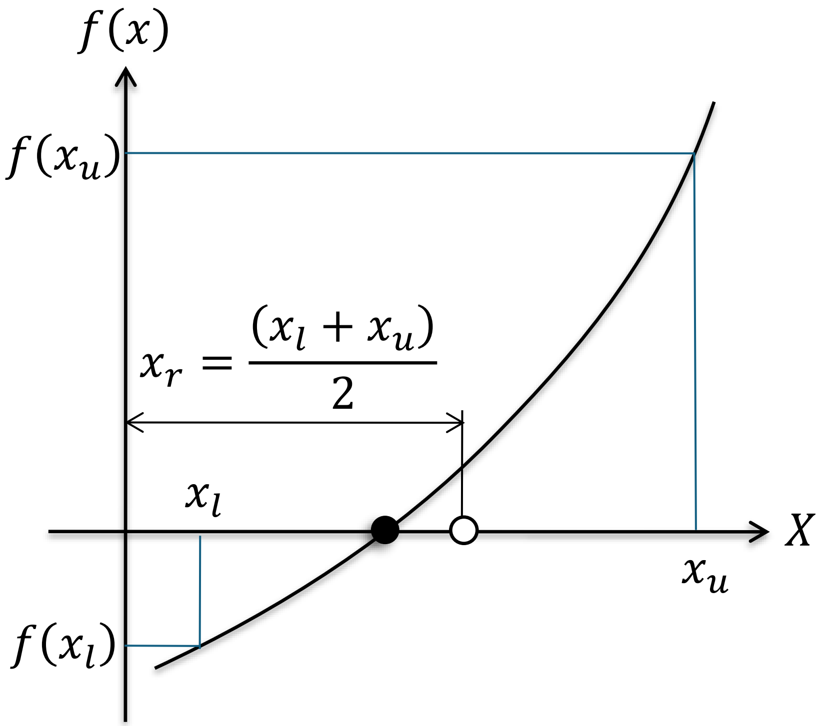




The false-position method

$f(x) = 0$

- Pitfalls of the bisection method
  - in dividing the interval from x_l to x_u into equal halves, no account is taken of the magnitudes of $f(x_l)$ and $f(x_u)$
  - if $f(x_l)$ is much closer to zero than $f(x_u)$, it is likely that the root is closer to x_l than to c_u

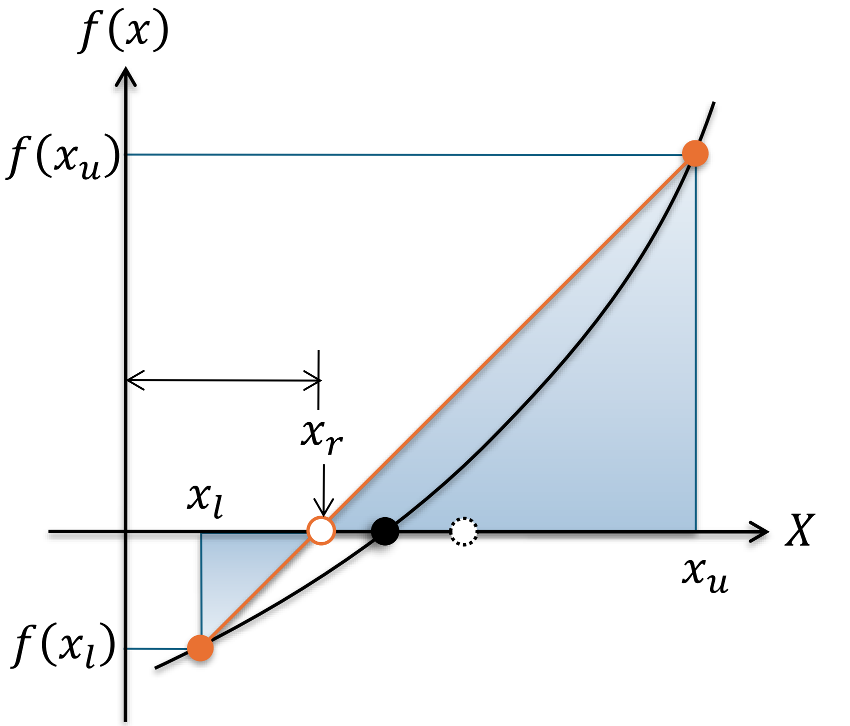


The false-position method

- Apply a straight line joining $f(x_l)$ and $f(x_u)$
  - apply a straight line joining $f(x_l)$ and $f(x_u)$
  - the intersection of this line with the x axis represents an improved estimate of the root
  - thus, x_r is

$$\frac{f(x_l)}{x_r - x_l} = \frac{f(x_u)}{x_r - x_u}$$

$$x_r = x_u - \frac{f(x_u)}{f(x_l) - f(x_u)}(x_l - x_u)$$

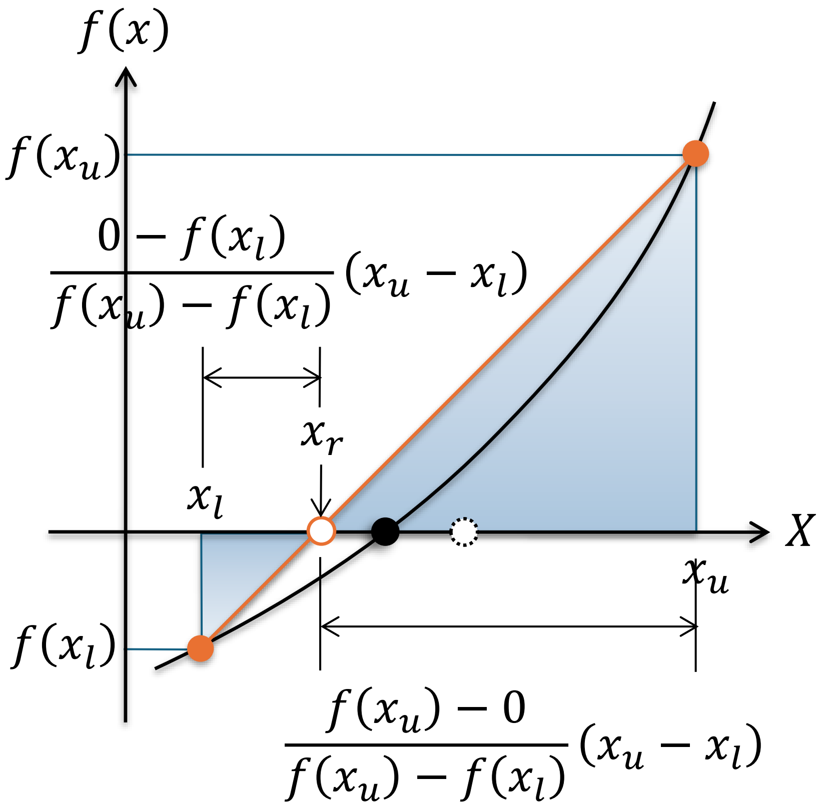


The false-position method

$$x_r = x_l - \frac{f(x_l)}{f(x_u) - f(x_l)}(x_u - x_l)$$

$$x_r = x_u - \frac{f(x_u)}{f(x_u) - f(x_l)}(x_u - x_l)$$

$$x_r = x_u - \frac{f(x_u)}{f(x_l) - f(x_u)}(x_l - x_u)$$



The false-position method

$$\epsilon_a = \left|\frac{c_r^{new} - c_r^{old}}{c_r^{new}}\right| 100\%$$

i	c_i	$f(c_i)$	c_r	Δc_r	ϵ_a (%)
0	12	6.0669			
1	16	-2.2688	14.9113		
2	14.9113	-0.2543	14.7942	-0.1171	0.7916
3	14.7942	-0.0273	14.7817	-0.0125	0.0845
4	14.7817	-0.0029	14.7823	0.0006	0.0039

- The above calculation table is compact but it may not be easily readable
- The following table is longer than this one, but it is more readable than the above table
- Note that the drag coefficient, c, is in kg/s unit and the function $f(c)$ is in m/s unit

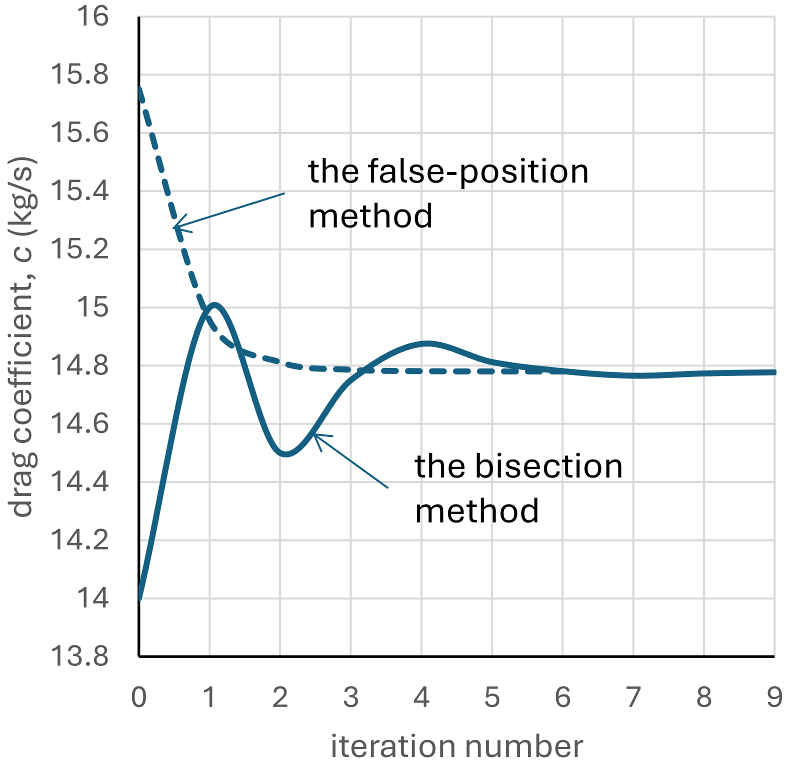
The false-position method

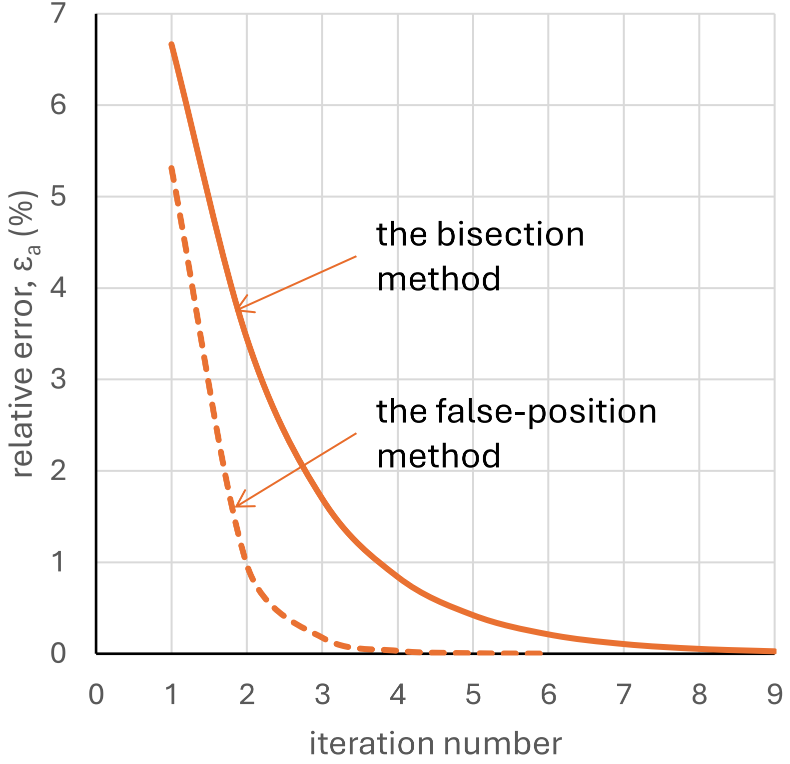
$$\epsilon_a = \left|\frac{c_r^{new} - c_r^{old}}{c_r^{new}}\right| 100\%$$

i	c_l	$f(c_l)$	c_u	$f(c_u)$	c_r	$f(c_r)$	$f(c_l)f(c_r)$	ϵ_a (%)
0	10	11.3691	20	-8.4006	15.7508	-81.6816	-928.647	
1	10	11.3691	15.7508	-1.8224	14.9563	-250.159	-2844.08	5.3120
2	10	11.3691	14.9563	-0.3409	14.8120	-1202.33	-13669.4	0.9742
3	10	11.3691	14.8120	-0.0619	14.7859	-6487.51	-73757.1	0.1762
4	10	11.3691	14.7859	-0.0112	14.7812	-35801.2	-407028	0.0318
5	10	11.3691	14.7812	-0.0020	14.7804	-198383	-2255434	0.0057
6	10	11.3691	14.7804	-0.0004	14.7802	-1100101	-1.3E+07	0.0010

$$f(c_{l,i-1})f(c_{r,i-1}) = \begin{cases} < 0 & \Longrightarrow c_{l,i} = c_{l,i-1} \wedge c_{u,i} = c_{r,i-1} \\ > 0 & \Longrightarrow c_{l,i} = c_{r,i-1} \wedge c_{u,i} = c_{u,i-1} \end{cases}$$

The bisection vs the false-position method



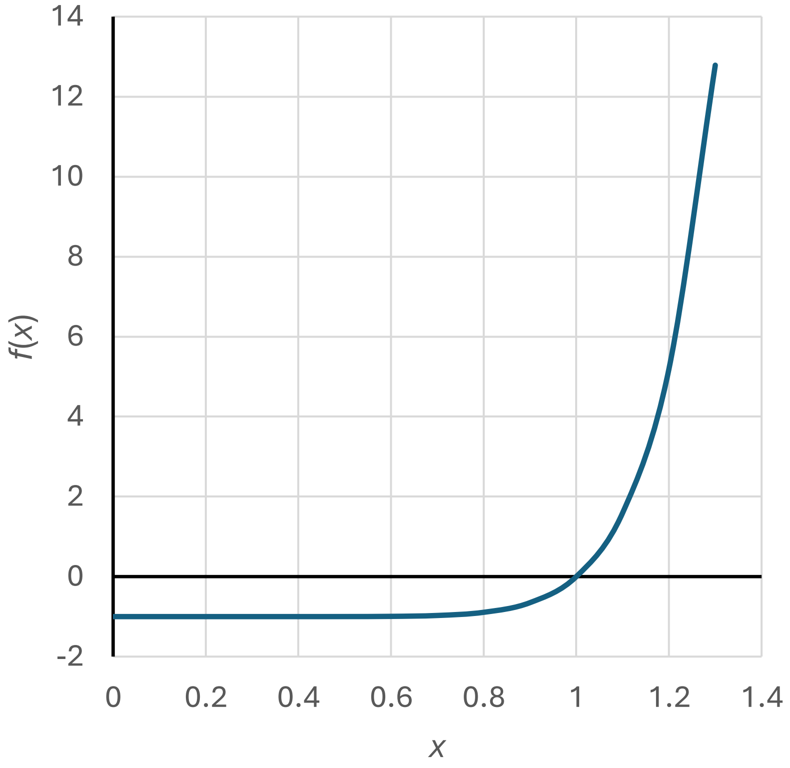


Pitfalls of the false-position method

- There are certain cases where bisection yields superior results.
- Example
  - Use bisection and false-position methods to locate the root of

    $$f(x) = x^{10} - 1$$

    between $x = 0$ and 1.3



Simple fixed-point iteration

$f(x) = 0$

- The method is known also as one-point iteration or successive substitution
- Steps
  1) rearrange the function $f(x) = 0$ so that x is on the left-hand side of the equation

     $$x = g(x)$$

  2) the transformation can be accomplished either by algebraic manipulation or by simply adding x to both sides of the original equation

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

     $$\sin x = 0 \quad \Leftrightarrow x = \sin x + x$$

Simple fixed-point iteration

- Steps
  3) given an initial guess at the root x_i, compute a new estimate x_{i+1} by an iterative formula

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

- The approximate error for this equation can be detemined using the error estimator

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

Simple fixed-point iteration

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

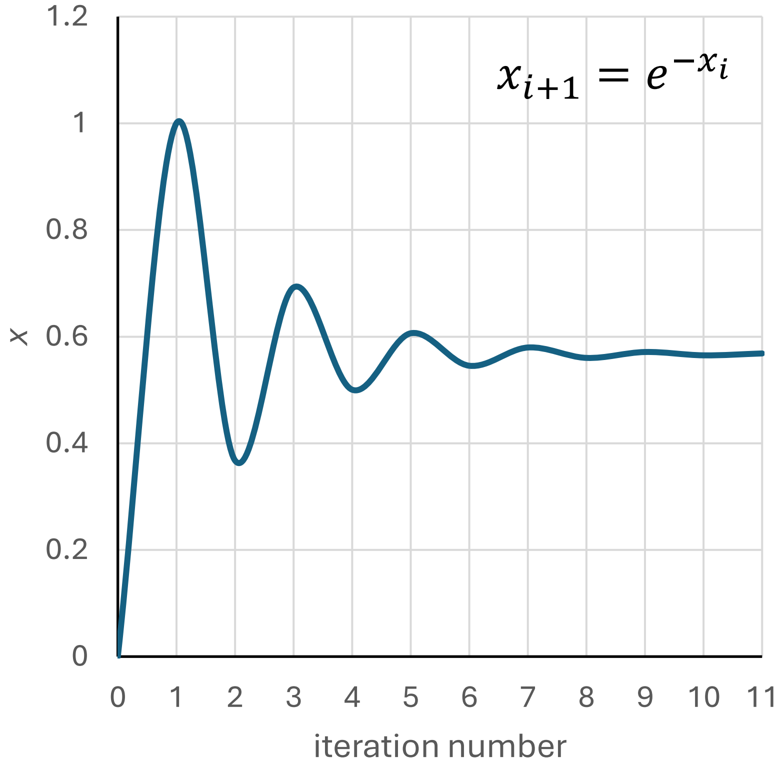
$$f(x) = e^{-x} - x \qquad \Longrightarrow x_{i+1} = e^{-x_i}$$

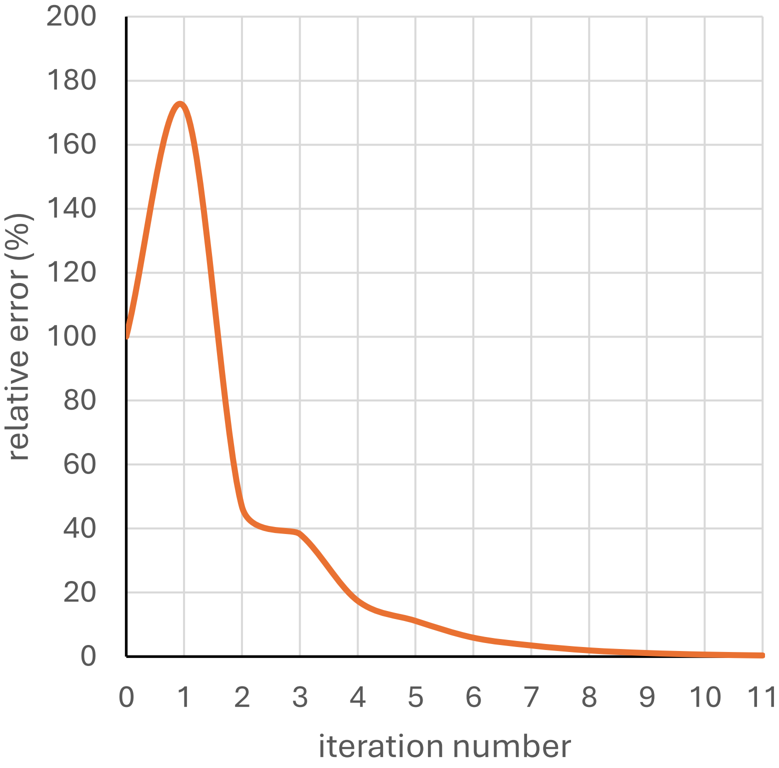
Simple fixed-point iteration

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

i	x_i	x_{i+1}	ϵ_a (%)
0	0	1	100
1	1	0.3679	171.8
2	0.3679	0.6922	46.9
3	0.6922	0.5005	38.3
4	0.5005	0.6062	17.4
5	0.6062	0.5454	11.2
6	0.5454	0.5796	5.9
7	0.5796	0.5601	3.5
8	0.5601	0.5711	1.9
9	0.5711	0.5649	1.1
10	0.5649	0.5684	0.6
11	0.5684	0.5664	0.4

Simple fixed-point iteration





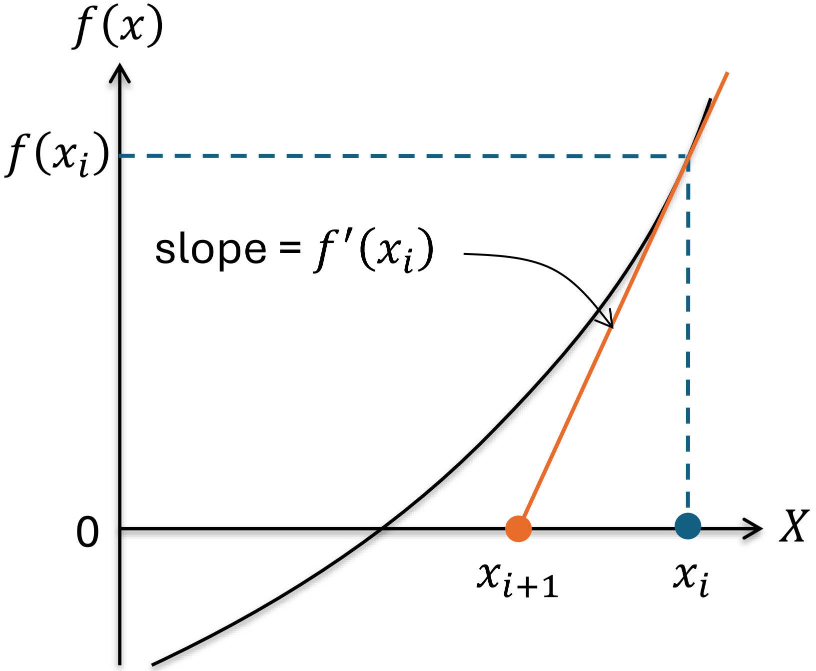
The Newton-Raphson method

$f(x) = 0$

- Steps
  1) find the first derivative $f'(x)$
  2) start with an initial guess x_i
  3) find the slope at point x_i, that is $f'(x_i)$
  4) compute the next estimate of the root x_{i+1} by

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

  5) iterate until convergence



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

The Newton-Raphson method

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

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

  - Substitute the first derivative along with the original function into the equation of the root estimate

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

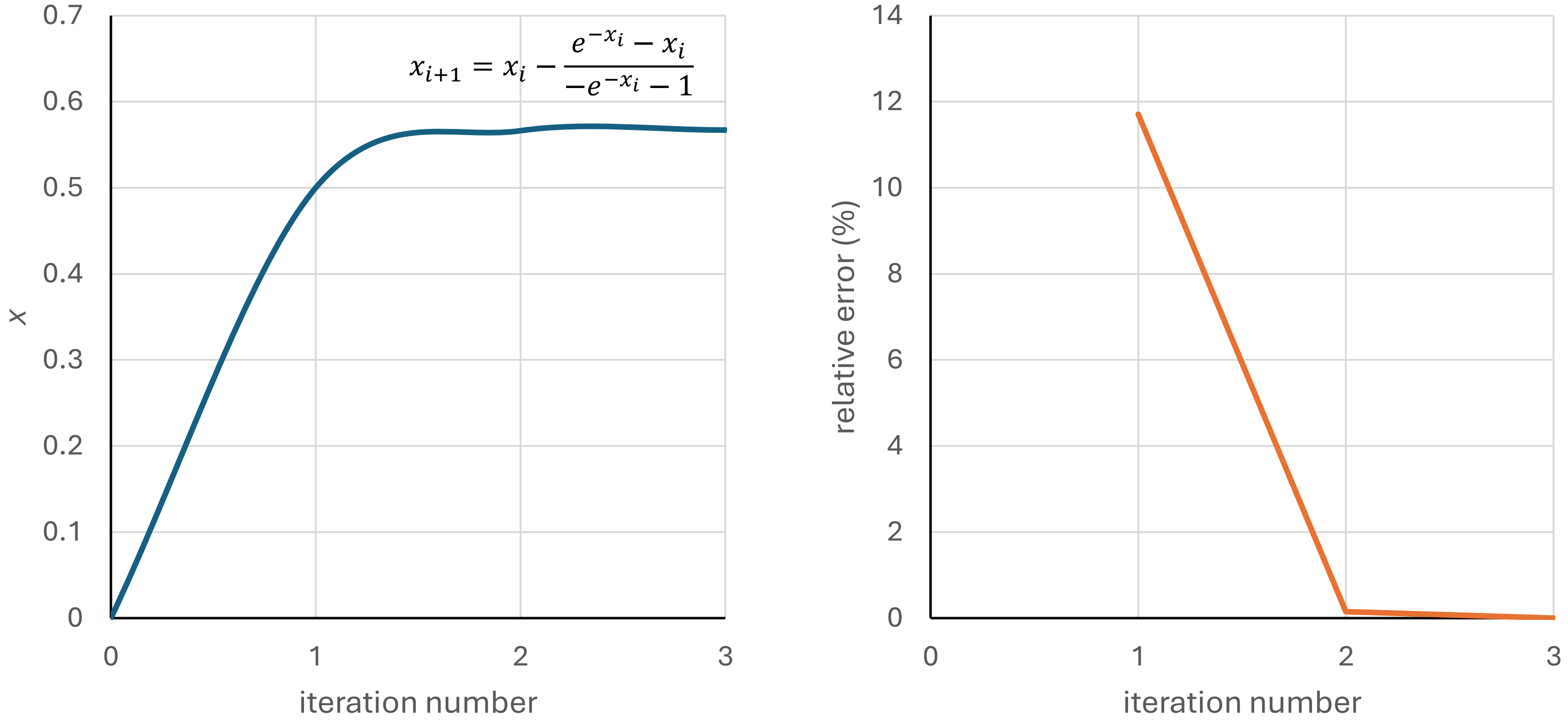
The Newton-Raphson method

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

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

i	x_i	$f(x_i)$	$f'(x_i)$	x_{i+1}	ϵ_a (%)
0	0	1	-2	0.5	
1	0.5	0.1065	-1.6065	0.5663	11.7093
2	0.5663	0.0013	-1.5676	0.5671	0.1467
3	0.5671	0.0000	-1.5671	0.5671	2.2E-05

The Newton-Raphson method



The Newton-Raphson method

- Pitfalls of the Newton-Raphson method
  - the first derivative of the function may be difficult to evaluate
  - the first derivative of the function may not exist
  - the iteration may exhibit slow convergence (large number of iterations)

↓

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

The Newton-Raphson method

Aside from slow convergence due to the nature of the function, other difficulties can arise, as illustrated in Fig. 6.6. For example, Fig. 6.6*a* depicts the case where an inflection point [that is, $f''(x) = 0$] occurs in the vicinity of a root. Notice that iterations beginning at x_0 progressively diverge from the root. Figure 6.6*b* illustrates the tendency of the Newton-Raphson technique to oscillate around a local maximum or minimum. Such oscillations may persist, or as in Fig. 6.6*b*, a near-zero slope is reached, whereupon the solution is sent far from the area of interest. Figure 6.6*c* 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. Obviously, a zero slope [$f'(x) = 0$] is truly a disaster because it causes division by zero in the Newton-Raphson formula [Eq. (6.6)]. Graphically (see Fig 6.6*d*), it means that the solution shoots off horizontally and never hits the x axis.

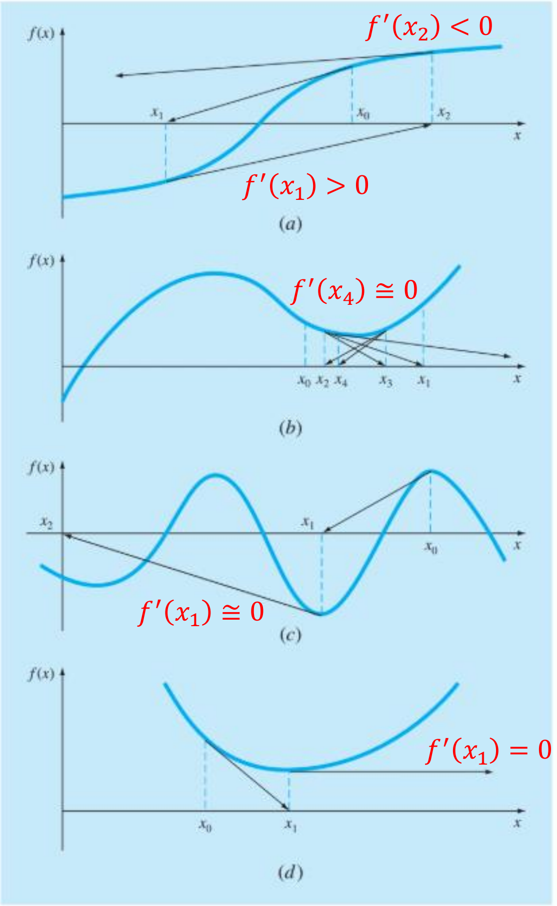


FIGURE 6.6
Four cases where the Newton-Raphson method exhibits poor convergence.

The secant method

$f(x) = 0$

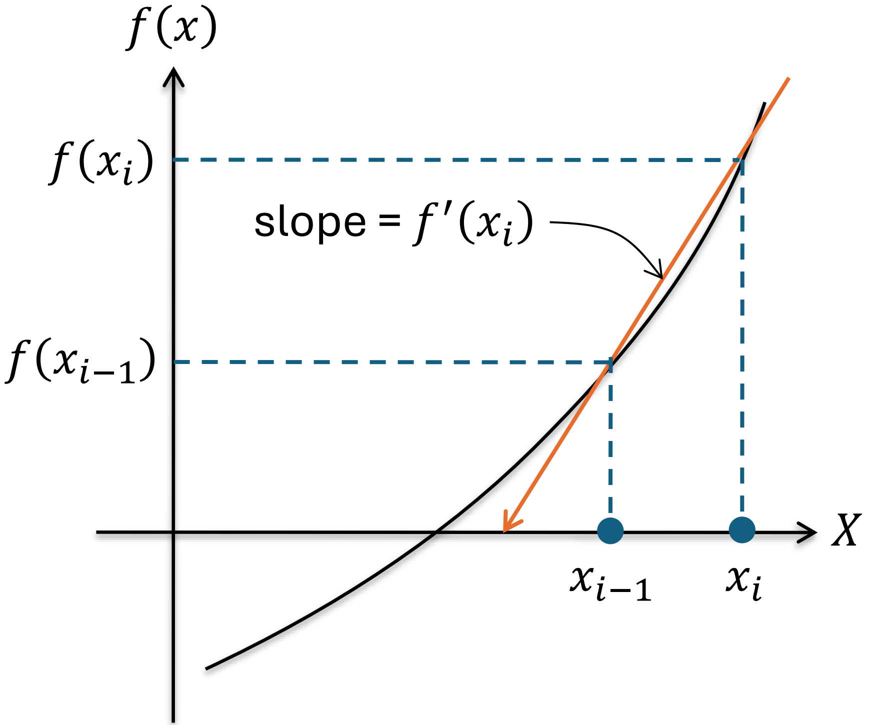
- Steps
  1) start with two initial estimates of x
  2) the derivative is approximated by a backward finite divided difference

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

  3) compute the next estimate of the root x_{i+1}

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

  4) iterate until convergence



requires two initial estimates of x

The secant method

- Problem statement
  - use the secant method to estimate the root of $f(x) = e^{-x} - x$
  - start with initial estimates of $x_{-1} = 0$ and $x_0 = 1$
- Solution
  - The first derivative of the function can be evaluated as

$$f'(x_{-1,0}) \cong \frac{f(x_{-1}) - f(x_0)}{x_{-1} - x_0} = \frac{f(0) - f(1)}{0 - 1} = \frac{(e^{-0} - 0) - (e^{-1} - 1)}{0 - 1} = 2 - e^{-1}$$

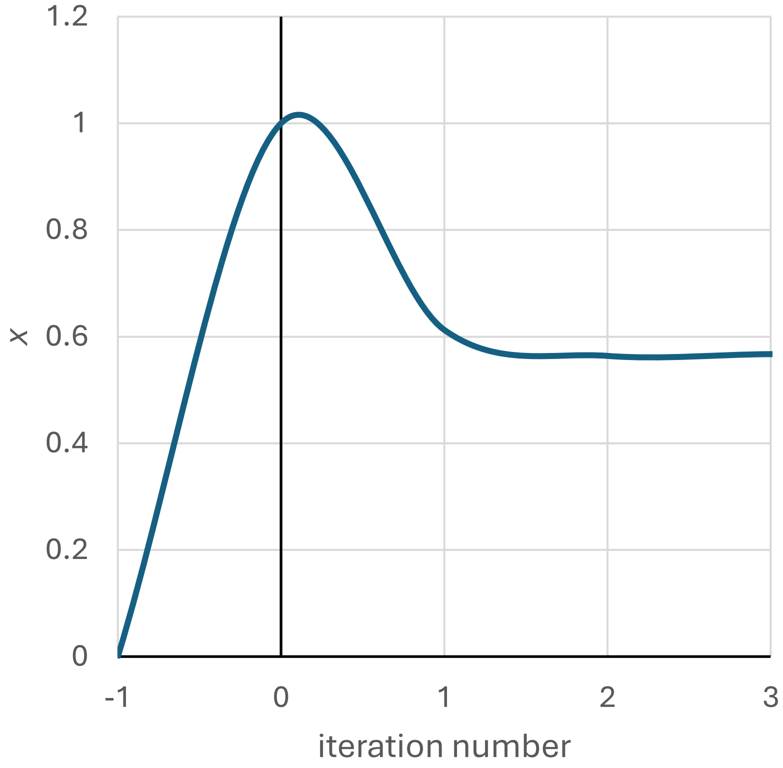
  - Substitute the first derivative along with the original function into the equation of the root estimate

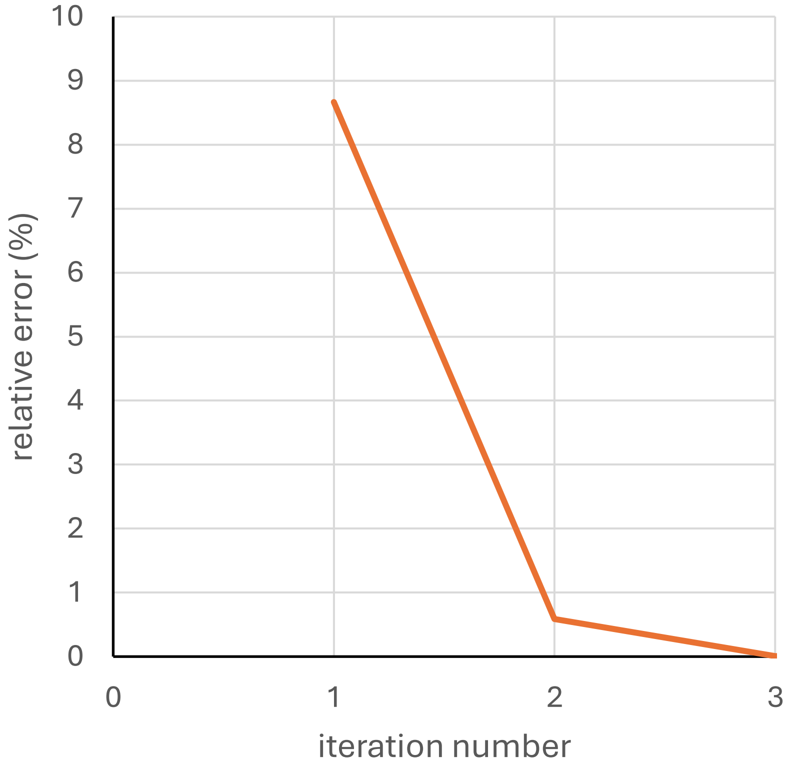
$$x_1 = x_0 - \frac{f(x_0)}{f'(x_{-1,0})} \quad \Leftrightarrow x_1 = 1 - \frac{e^{-1} - 1}{2 - e^{-1}} = 0.6127$$

The secant method

i	x_i	$f(x_i)$	$f'(x_i)$	x_{i+1}	ϵ_a (%)
-1	0	1			
0	1	-0.6321	-1.6321	0.6127	
1	0.6127	-0.0708	-1.4493	0.5638	8.6659
2	0.5638	0.0052	-1.5553	0.5672	0.5875
3	0.5672	0.0000	-1.5681	0.5671	0.0048
4	0.5671	0.0000	-1.5671	0.5671	0.0000

The secant method





Multiple roots

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

$$f(x) = (x-3)(x-1)(x-1)$$
$$\Leftrightarrow f(x) = x^3 - 5x^2 + 7x - 3$$

  - example: a triple root results from

$$f(x) = (x-3)(x-1)(x-1)(x-1)$$
$$\Leftrightarrow f(x) = x^4 - 6x^3 + 12x^2 - 10x + 3$$

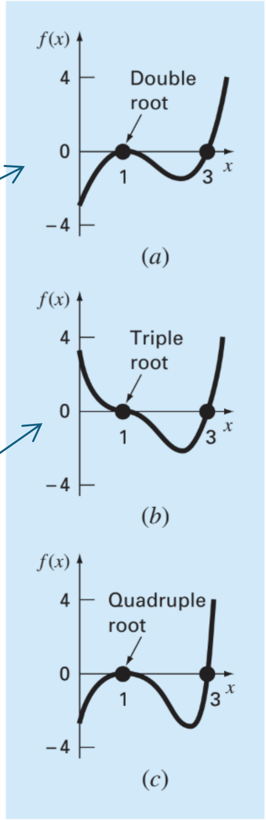


FIGURE 6.13
Examples of multiple roots that are tangential to the x axis. Notice that the function does not cross the axis on either side of even multiple roots (a) and (c), whereas it crosses the axis for odd cases (b).

Multiple roots

- Modified Newton-Raphson method

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

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

it can be shown that this function, $u(x)$, has roots at all the same locations as the original function, $f(x)$

differentiation

$$u'(x) = \frac{f'(x)f'^{(x)} - f(x)f''(x)}{[f'(x)]^2}$$

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

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

Multiple roots

- Problem statement
  - Use both the standard and modified Newton-Raphson methods to evaluate the multiple root of

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

  - with an initial guess of $x_0 = 0$
- Solution

$$f(x) = x^3 - 5x^2 + 7x - 3$$

$$f'(x) = 3x^2 - 10x + 7$$

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

the NR method

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

the modified NR method

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

Multiple roots

The Newton-Raphson method

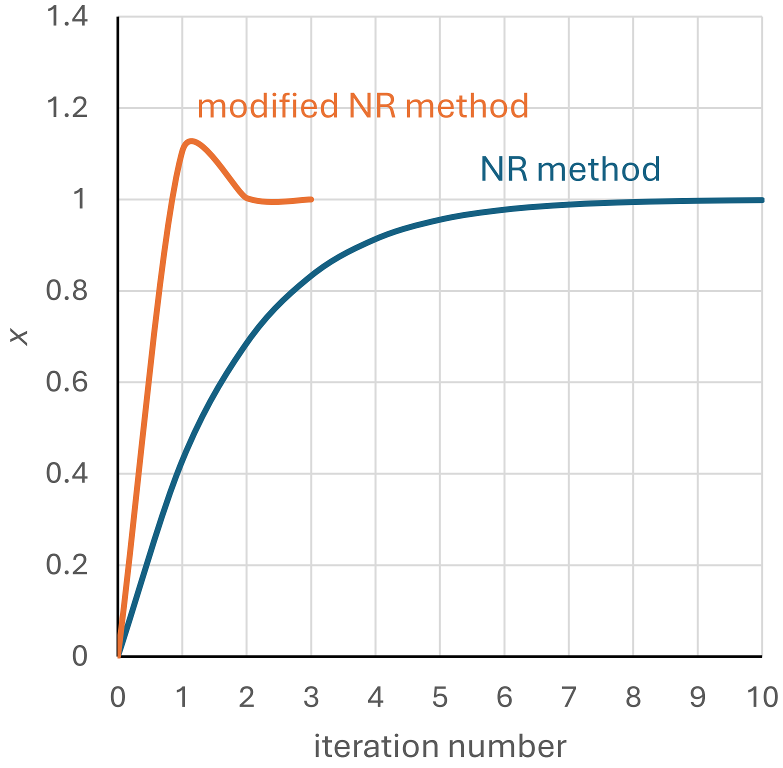
i	x_i	$f(x_i)$	$f'(x_i)$	x_{i+1}	ϵ_a (%)
0	0	-3	7	0.428571	
1	0.4286	-0.8397	3.2653	0.6857	37.50
2	0.6857	-0.2286	1.5535	0.8329	17.67
3	0.8329	-0.0605	0.7523	0.9133	8.81
4	0.9133	-0.0157	0.3692	0.9558	4.44
5	0.9558	-0.0040	0.1827	0.9777	2.24
6	0.9777	-0.0010	0.0909	0.9888	1.12
7	0.9888	-0.0003	0.0453	0.9944	0.56
8	0.9944	-0.0001	0.0226	0.9972	0.28
9	0.9972	0.0000	0.0113	0.9986	0.14
10	0.9986	0.0000	0.0057	0.9993	0.07

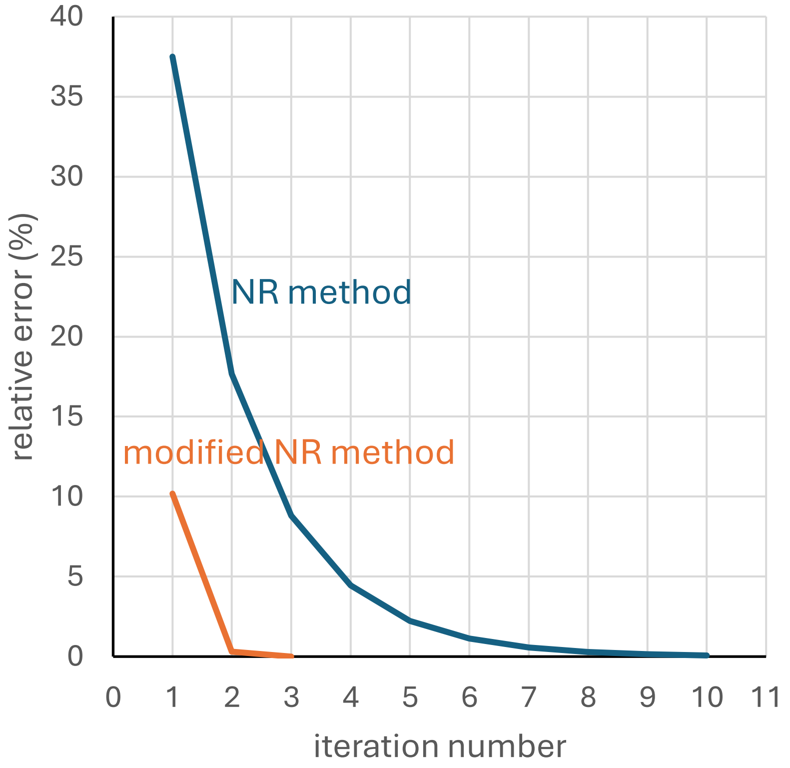
Multiple roots

The modified Newton-Raphson method

i	x_i	$f(x_i)$	$f'(x_i)$	$f''(x_i)$	x_{i+1}	ϵ_a (%)
0	0	-3	7	-10	1.105263	
1	1.1053	-0.0210	-0.3878	-3.36842	1.003082	10.1868
2	1.0031	0.0000	-0.0123	-3.98151	1.000002	0.3079
3	1.0000	0.0000	0.0000	-3.99999	1	0.0002

Multiple roots





Numerical Methods

Roots of Equations