Solving equations – Root finding

Introduction to Numerical Problem Solving, Spring 2017

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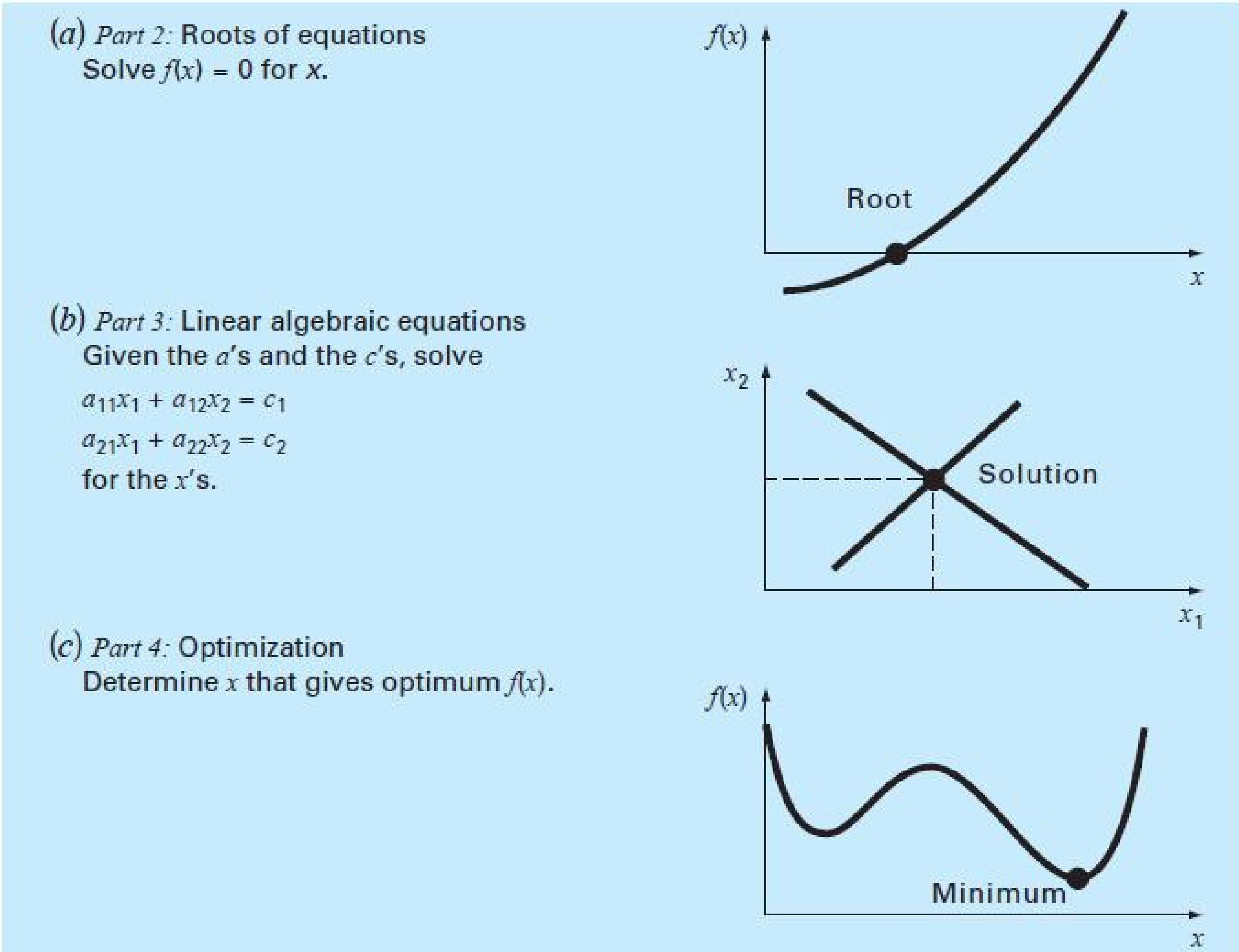
Review of numerical methods (1)

Next

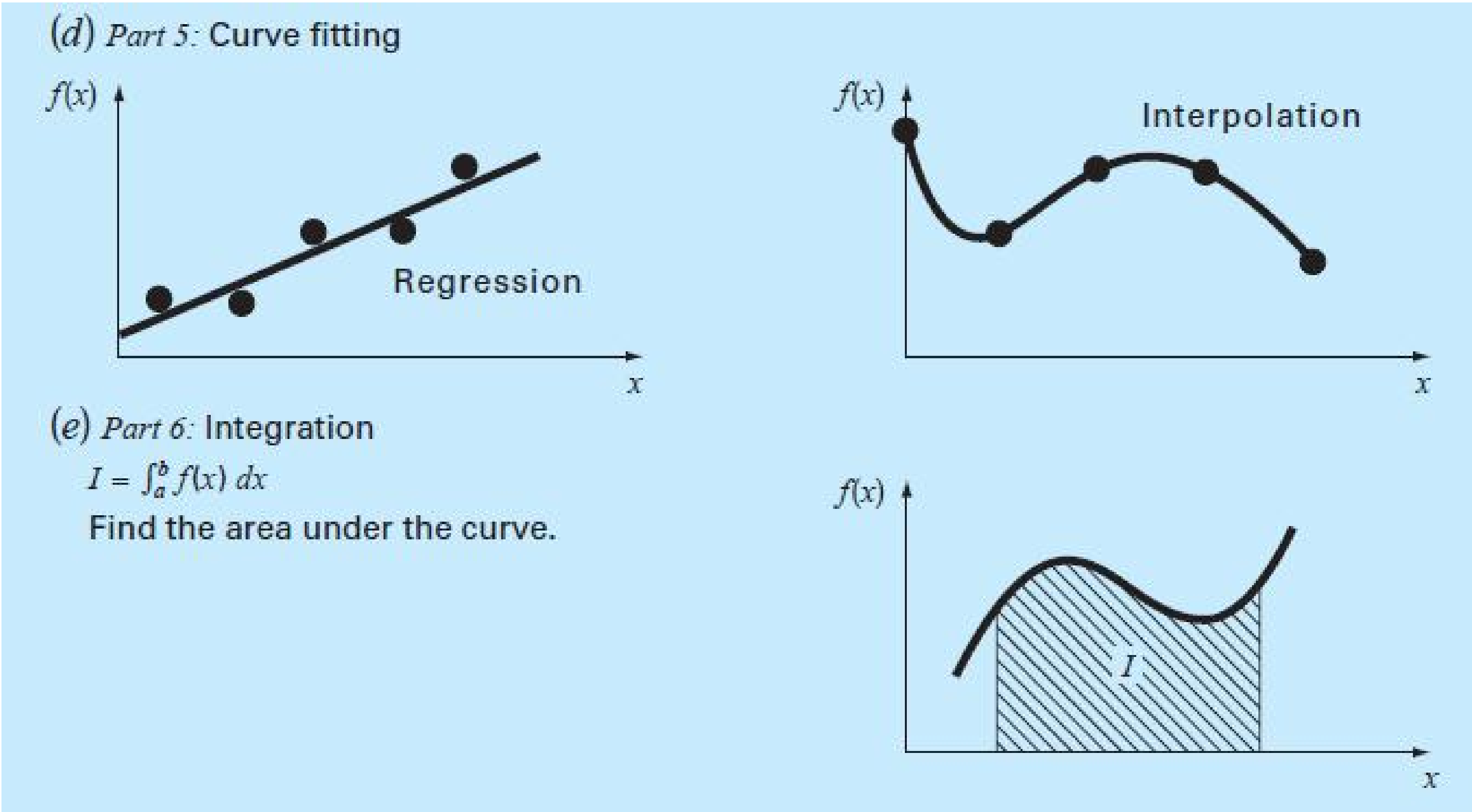
Done!

Later



Chapra & Canale. (2010). p. 6.

Review of numerical methods (2)



Chapra & Canale. (2010). p. 6.

Review of numerical methods (3)

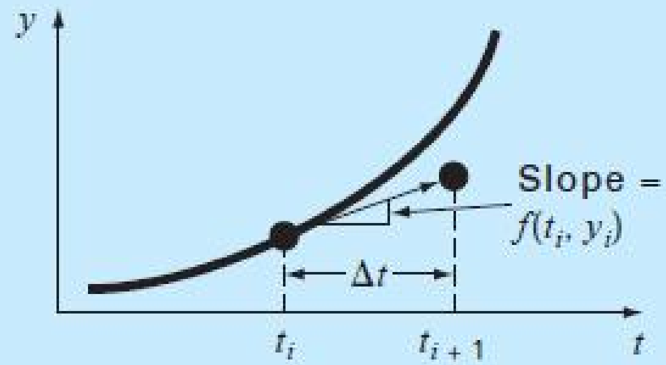
(*f*) *Part 7:* Ordinary differential equations

Given

$$\frac{dy}{dt} \cong \frac{\Delta y}{\Delta t} = f(t, y)$$

solve for y as a function of t.

$$y_{i+1} = y_i + f(t_i, y_i)\,\Delta t$$

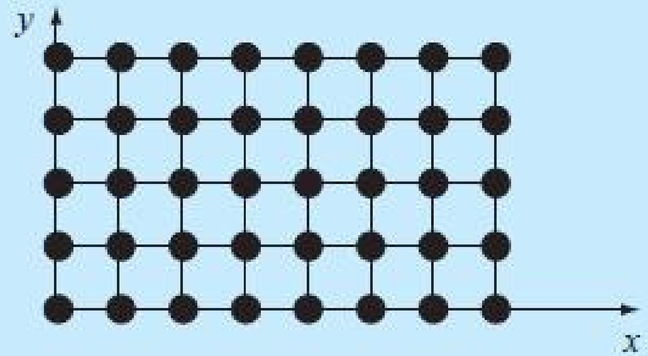


(*g*) *Part 8:* Partial differential equations

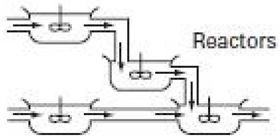
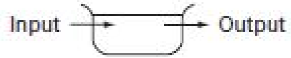
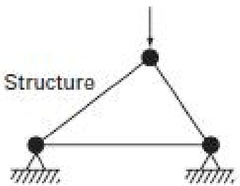
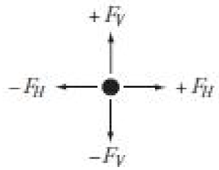
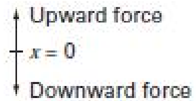
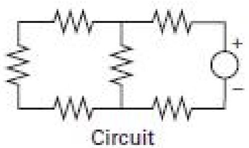
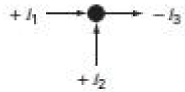
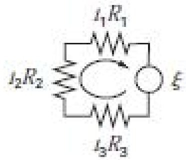
Given

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$$

solve for u as a function of x and y



Chapra & Canale. (2010). p. 6.

Field	Device	Organizing Principle	Mathematical Expression
Chemical engineering		Conservation of mass	Mass balance:  Over a unit of time period Δmass = inputs − outputs
Civil engineering		Conservation of momentum	Force balance:  At each node Σ horizontal forces (F_H) = 0 Σ vertical forces (F_V) = 0
Mechanical engineering		Conservation of momentum	Force balance:  $m\frac{d^2x}{dt^2}$ = downward force − upward force
Electrical engineering		Conservation of charge	Current balance: For each node Σ current (i) = 0 
		Conservation of energy	Voltage balance:  Around each loop Σ emf's − Σ voltage drops for resistors = 0 $\Sigma\xi - \Sigma iR = 0$

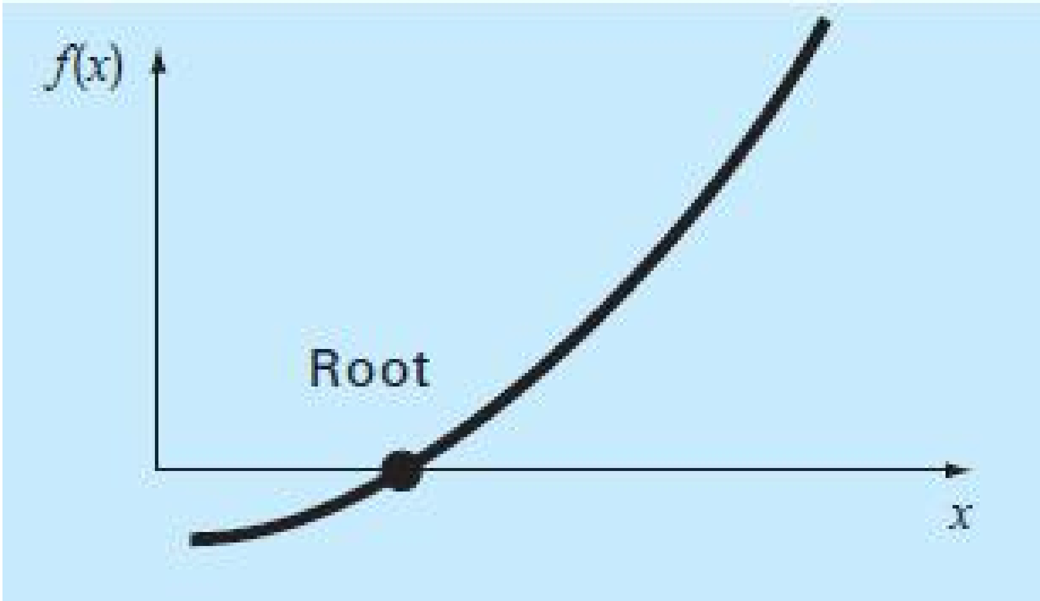
Four (five) major areas of engineering

1. Civil engineering
2. Mechanical engineering
3. Chemical engineering
4. Electrical engineering

(5. IT engineering)

Chapra & Canale. (2010). p. 20.

Problem



Find the solutions of $f(x) = 0$, where the function $f(x)$ is known.

Motivation – Why numerical solutions?

How often do you have an analytical solution for f(x) = 0?

$$f(x) = ax^2 + bx + c = 0 \quad \Rightarrow \quad x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$f(x) = e^{-x} - x \quad \Rightarrow \quad ?$$

Practical engineering problems

Parachuitist's velocity

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

What should be the drag constant c?

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

$f(c) = 0$ How to find c ?

Root finding methods

Bracketing methods

- Graphical
- Incremental search
- Bisection
- False position

Open methods

- Simple fixed point iteration
- Newton-Raphson
- Secant
- Modified secant

Hybrid

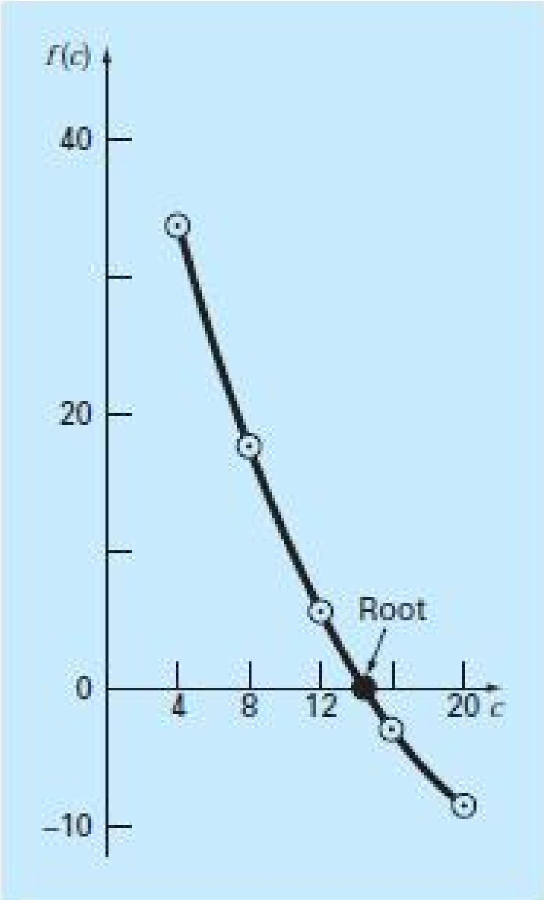
- Brent

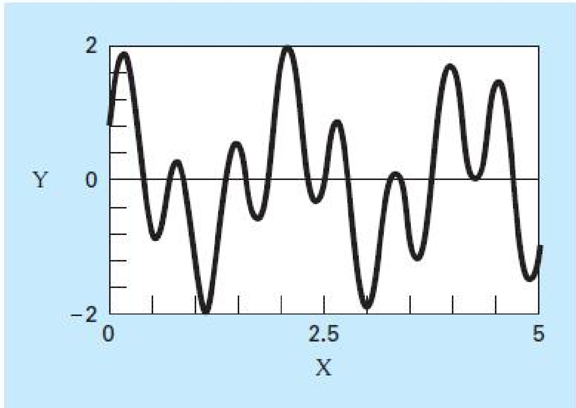
Bracketing methods

Find $f(x) = 0$ when we know that

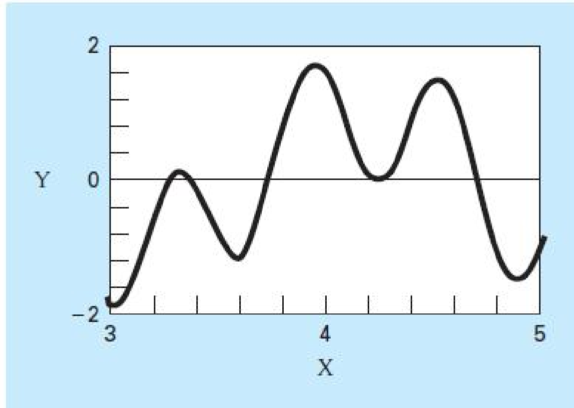
there is at least one root between the brackets $[a, b]$

Graphical method (progressive zooming)

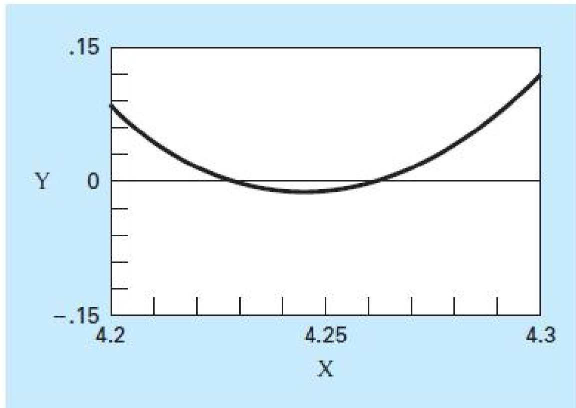




(a)

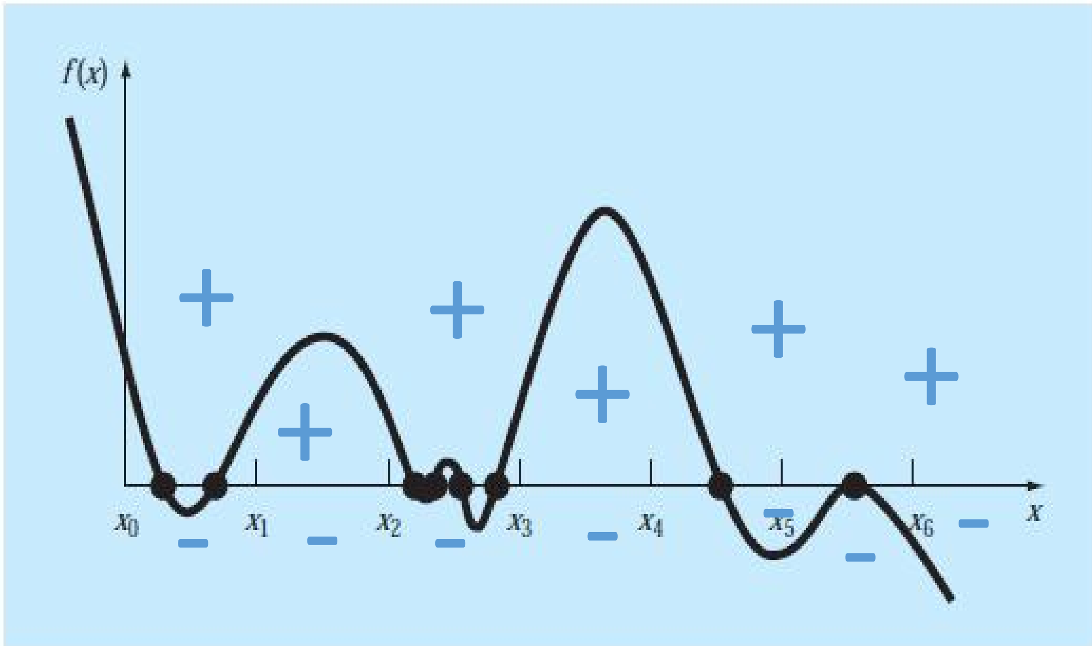


(b)



Incremental search (determining initial guesses)

```
x = a
while x < b:
   x = x + dx
   if sign(f(x)) != sign(f(x + dx)):
      return x, x + dx
```



Bisection search

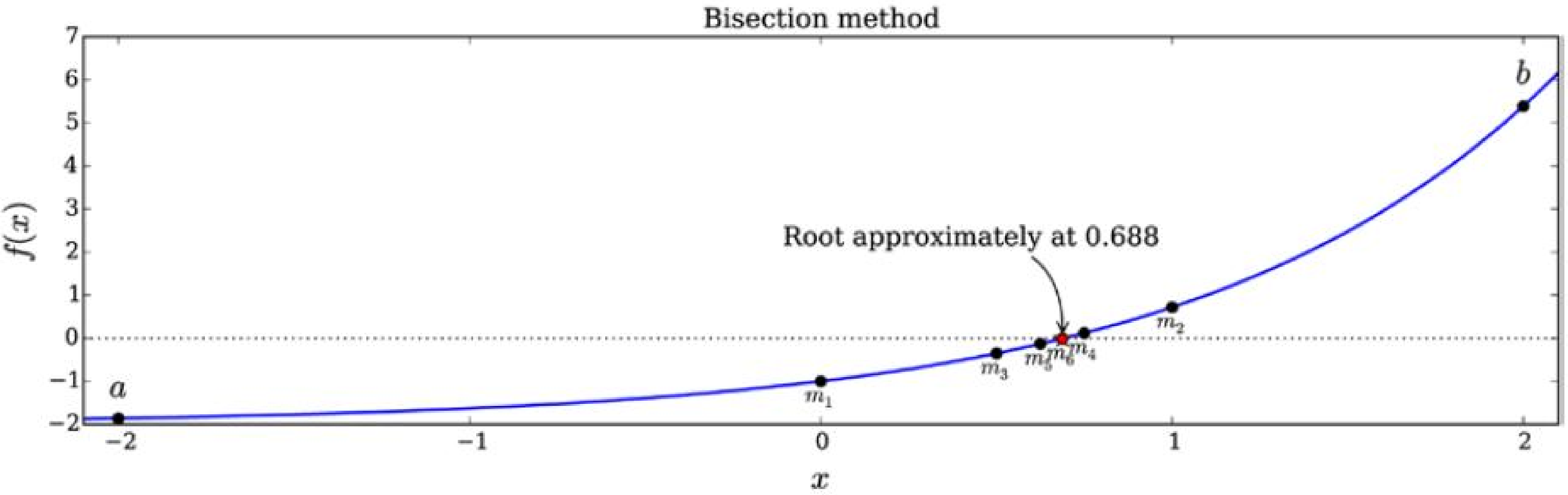
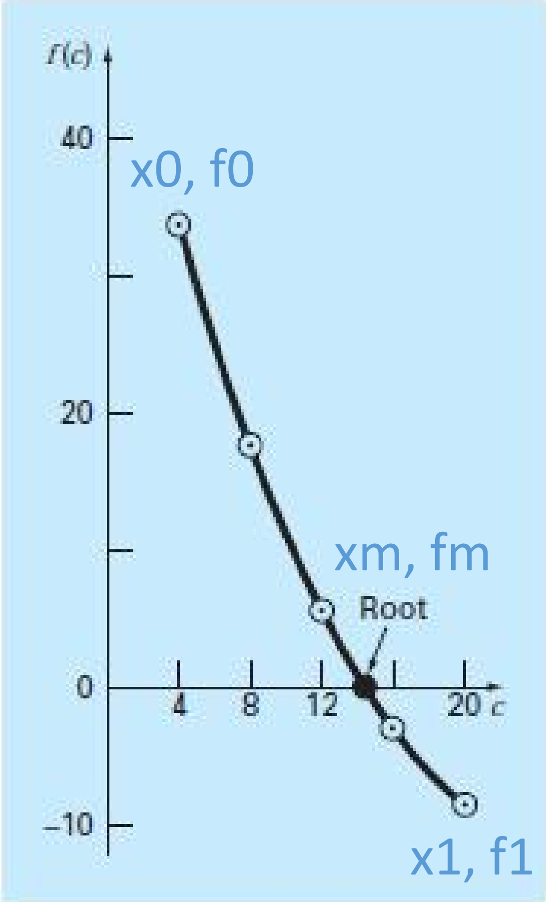


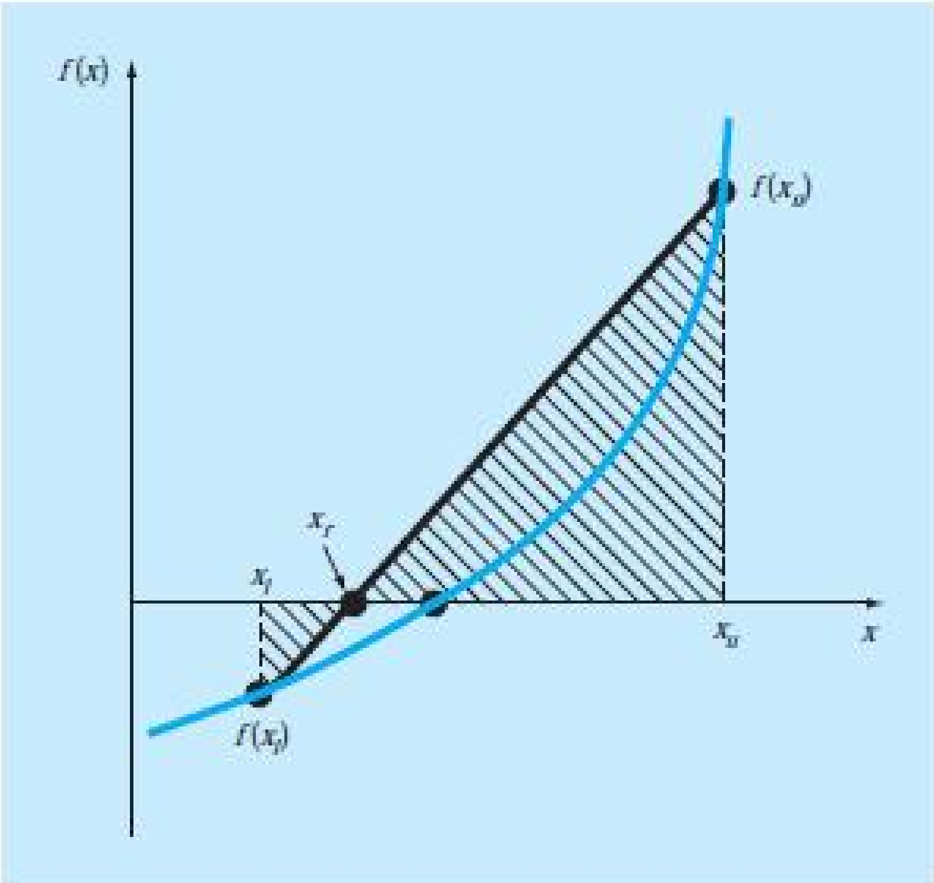
Figure 5-6. *Graphical visualization of how the bisection method works*

Bisection search algorithm

```
# Initial values
x0, x1 = a, b
f0, f1 = f(x0), f(x1)
# Loop until max iterations
while n < nmax:
   xm = (x0 + x1)/2
   fm = f(xm)
   # Change the brackets
   if sign(fm) == sign(f0):
       x0, f0 = xm, fm
   else:
       x1, f1 = xm, fm
   # Stop criteria
   ea = …
   if ea < etol:
      return xm
```



The False position method



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

which can be solved for (see Box 5.1 for details).

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

Stop criteria: $\epsilon_a < \epsilon_{tol}$

$$\varepsilon_a = \left| \frac{x_r^{\text{new}} - x_r^{\text{old}}}{x_r^{\text{new}}} \right| 100\%$$

Bisection vs. False position

$$f(c) = \frac{667.38}{c}\left(1 - e^{-0.146843c}\right) - 40$$

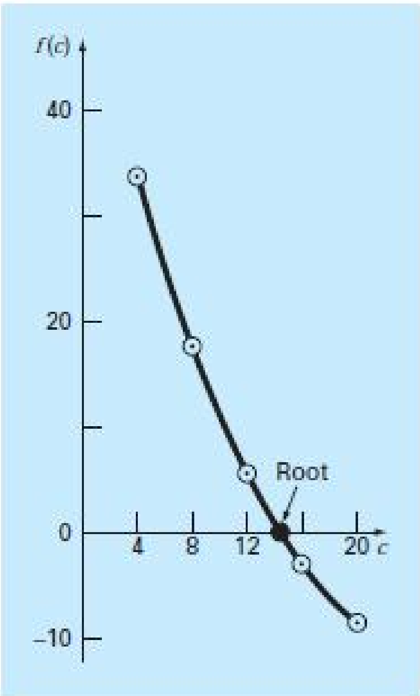
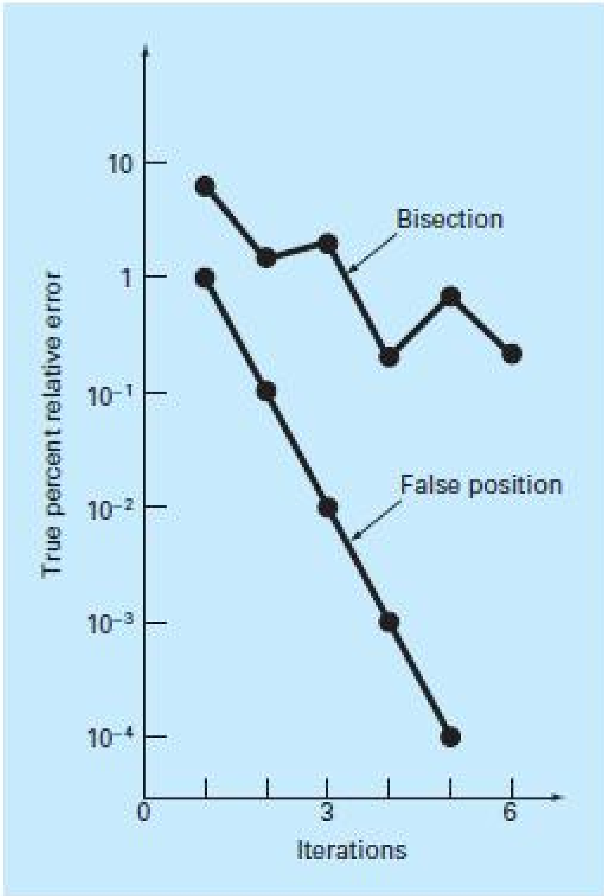


FIGURE 5.13
Comparison of the relative errors of the bisection and the false-position methods.



Pitfall of False position method

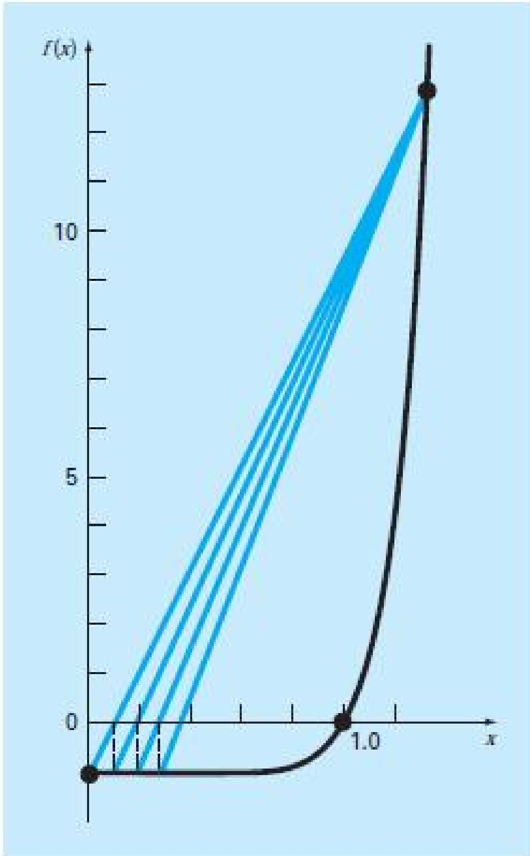


FIGURE 5.14
Plot of $f(x) = x^{10} - 1$, illustrating slow convergence of the false-position method.

Open methods

Find f(x) = 0 with initial guess x = x0

Simple Fixed-Point iteration

Rearrange the function f(x) = 0, so that the x is on the left-hand side

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

Relative approximation error

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

Stop criteria

$$\epsilon_a < \epsilon\_tol$$

Examples – rearrangements of the equation

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

Can be manipulated to yield

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

$$\sin(x) = 0$$

Adding x on both sides

$$x = \sin(x) + x$$

When does the fixed-point iteration converge?

Example: $f(x) = e^{-x} - x$

Rearranged: $x = e^{-x}$

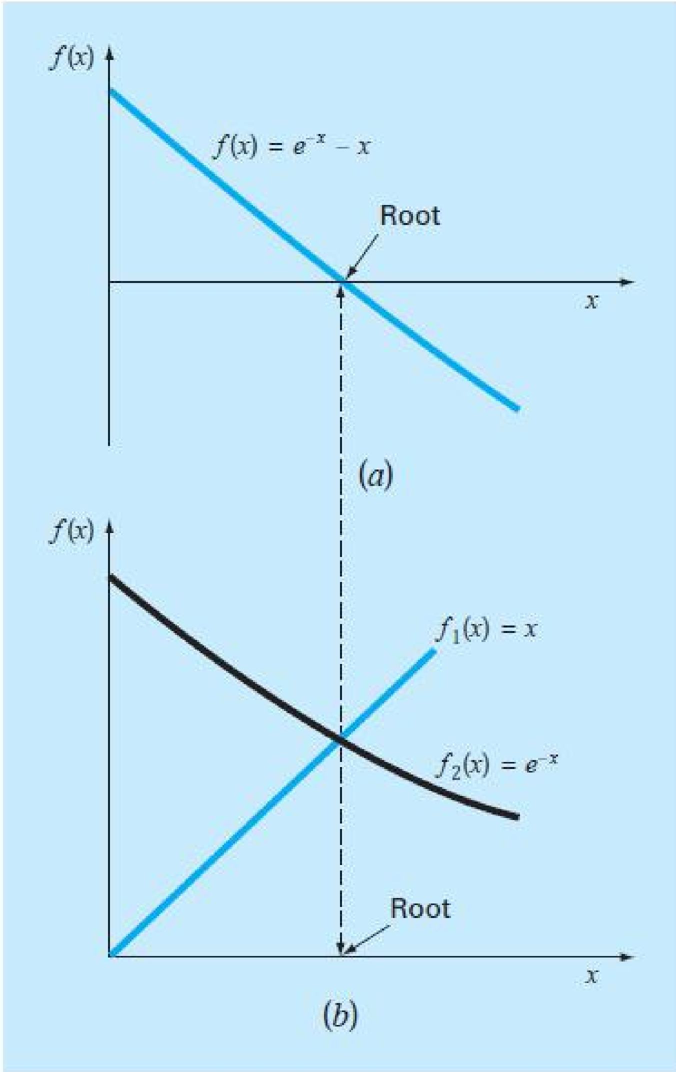
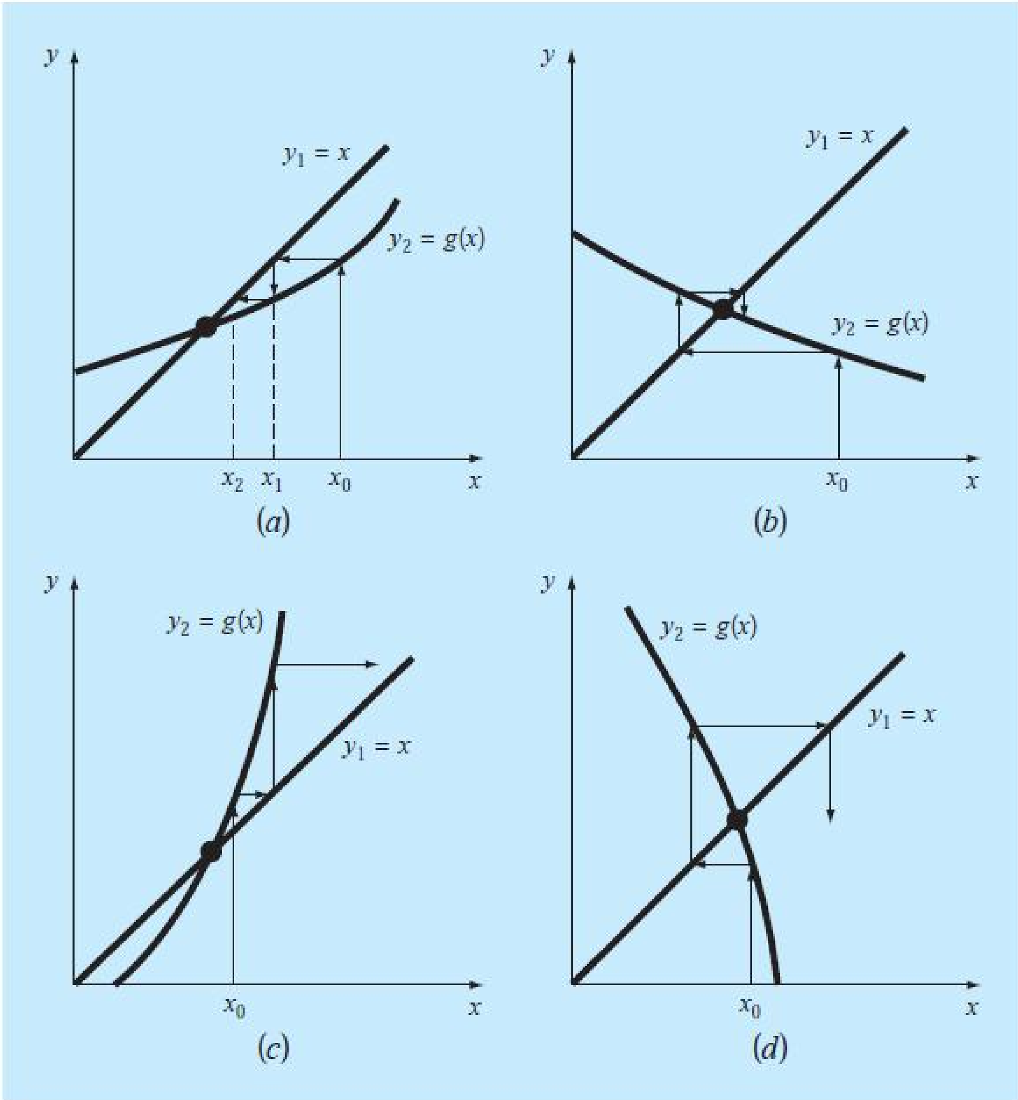


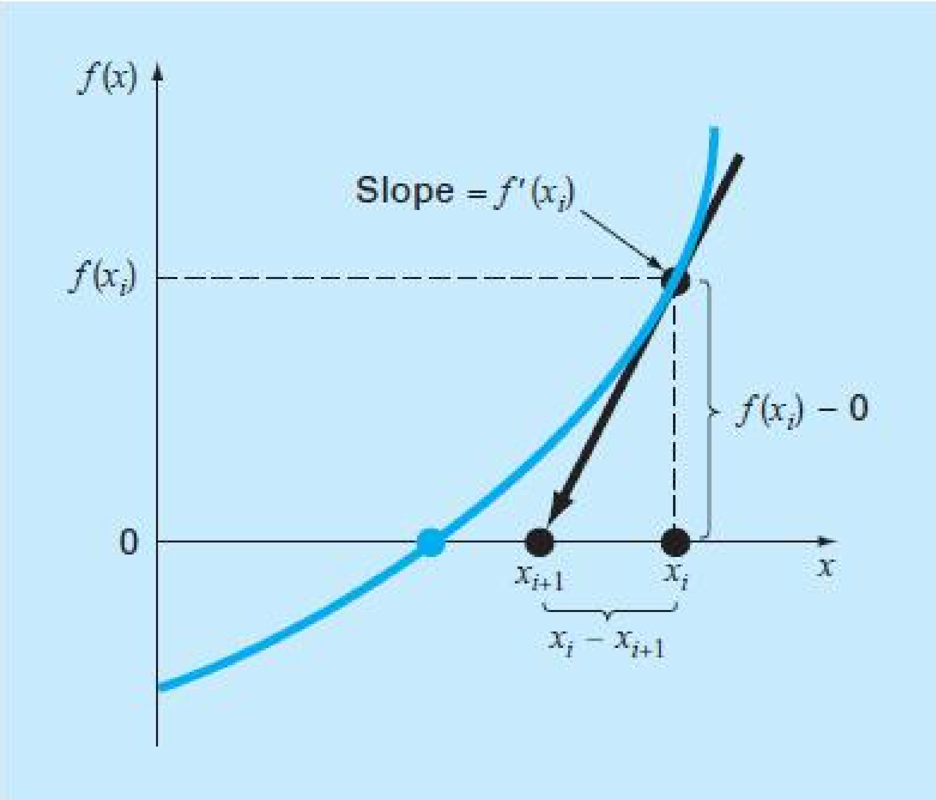
FIGURE 6.3
Graphical depiction of (*a*) and (*b*) convergence and (*c*) and (*d*) divergence of simple fixed-point iteration. Graphs (*a*) and (*c*) are called monotone patterns, whereas (*b*) and (*d*) are called oscillating or spiral patterns. Note that convergence occurs when $|g'(x)| < 1$.



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

$$|g'(x)| \geq 1$$

Newton-Raphson method
"follow the tangent line"



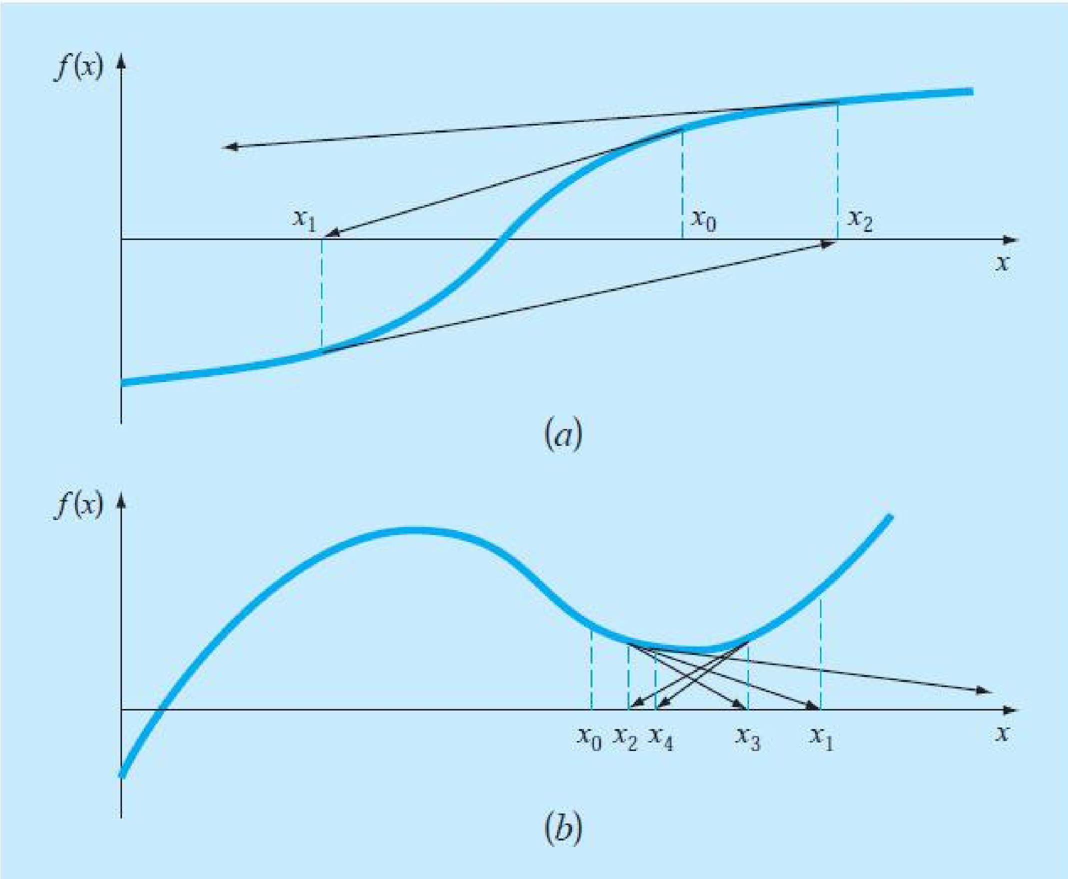
$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}}$$

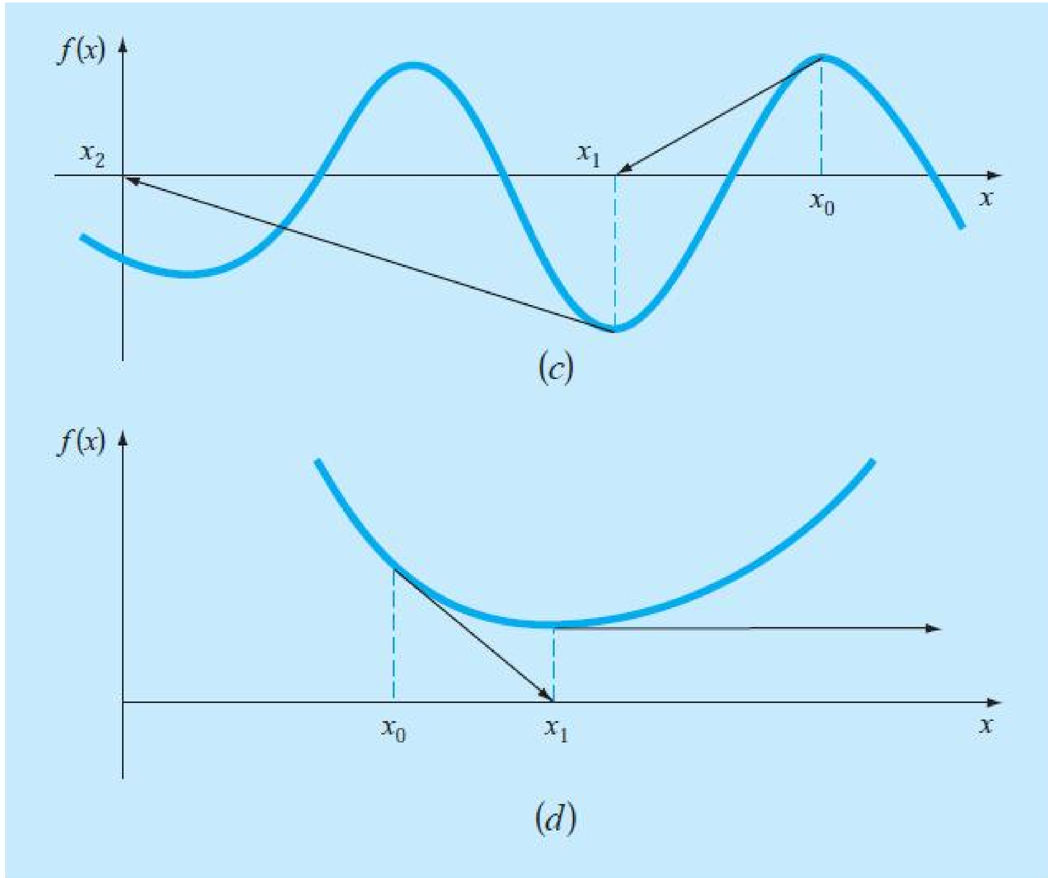
which can be rearranged to yield

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

which is called the *Newton-Raphson formula*.

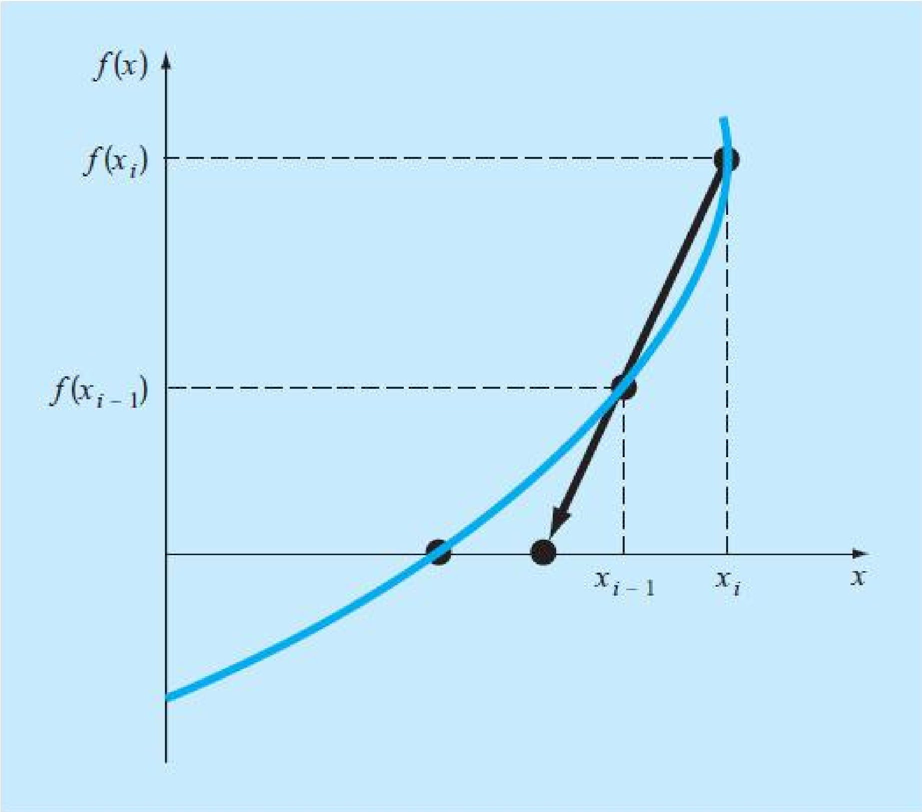
Pitfalls of Newton-Raphson method





Secant Method

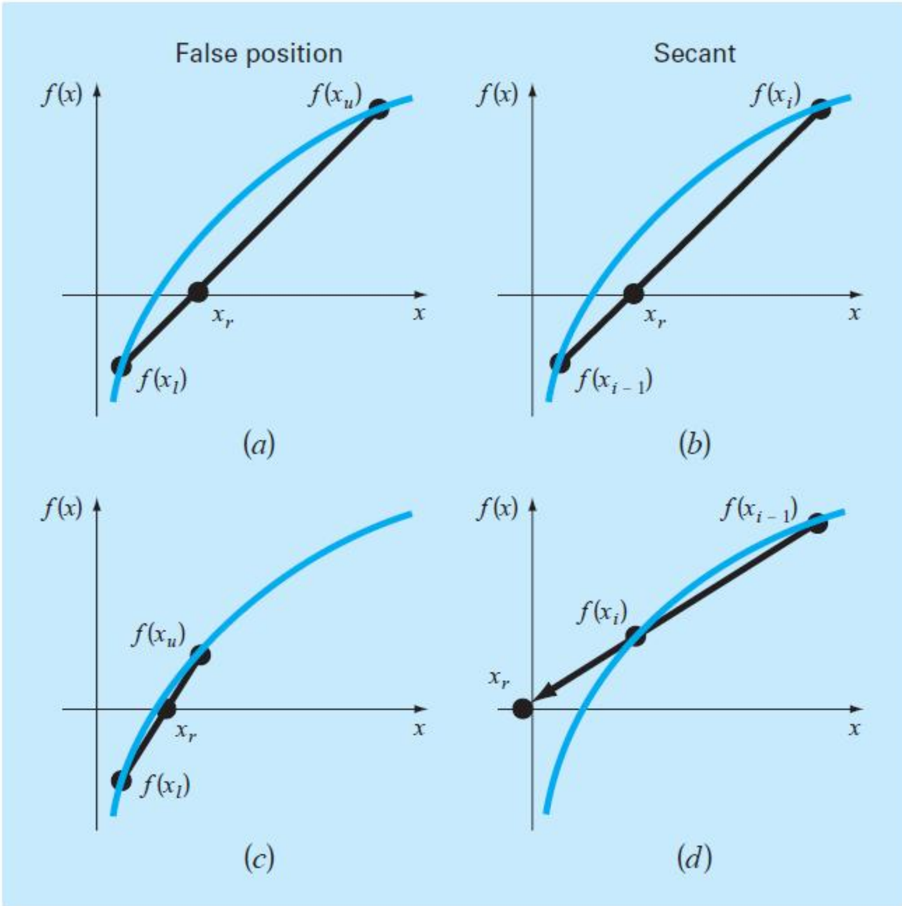
"draw a secant and follow it"



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

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

False position vs. Secant method



Modified secant method

Modified secant $f'(x_i) \cong \dfrac{f(x_i + \delta x_i) - f(x_i)}{\delta x_i}$

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

Newton-Raphson $f'(x_i)$ is known

Common to all $\boxed{x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x_i)}}$

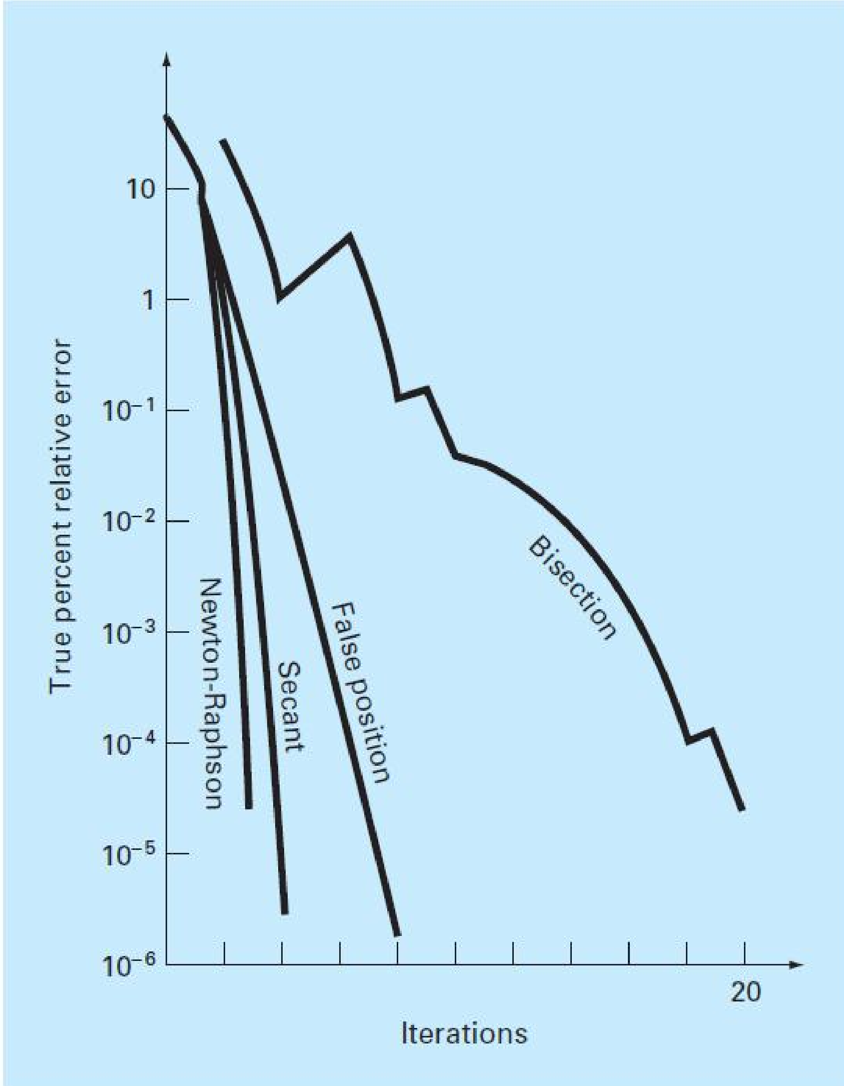
Comparison of Methods

True percent relative error for

1. Bisection,
2. False position,
3. Secant, and
4. Newton-Raphson method

to determine the roots of

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



Hybrid methods

- Hybrid methods like **Brent's method** use a speedy open method wherever possible, but reverts to a reliable bracketing method when necessary.

Scipy.org | Docs | SciPy v0.18.1 Reference Guide | Optimization and root finding (`scipy.optimize`) | index

scipy.optimize.brentq

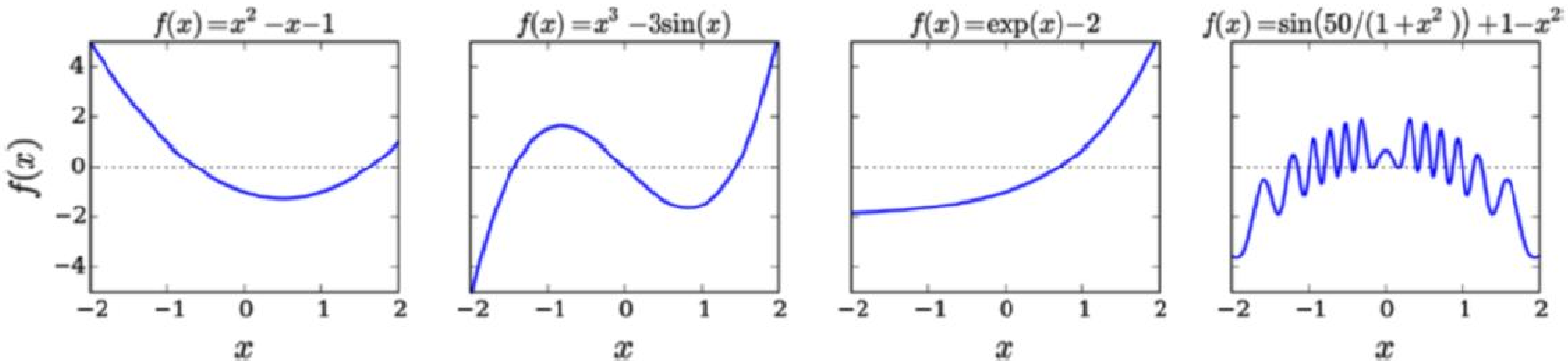
scipy.optimize.brentq(*f, a, b, args=(), xtol=2e-12, rtol=8.8817841970012523e-16, maxiter=100, full_output=False, disp=True*) [source]

Find a root of a function in a bracketing interval using Brent's method.

Uses the classic Brent's method to find a zero of the function *f* on the sign changing interval [a , b]. Generally considered the best of the rootfinding routines here. It is a safe version of the secant method that uses inverse quadratic extrapolation. Brent's method combines root bracketing, interval bisection, and inverse quadratic interpolation. It is sometimes known as the van Wijngaarden-Dekker-Brent method. Brent (1973) claims convergence is guaranteed for functions computable within [a,b].

[Brent1973] provides the classic description of the algorithm. Another description can be found in a recent edition of Numerical Recipes, including [PressEtal1992]. Another description is at http://mathworld.wolfram.com/BrentsMethod.html. It should be easy to understand the algorithm just by reading our code. Our code diverges a bit from standard presentations: we choose a different formula for the extrapolation step.

Exercises



Reference books

Chapra & Canale. (2010). Numerical Methods for Engineers, 6th edition.

Part two: Roots of equations.

Kiusalaas. (2013). Numerical Methods in Engineering with Python 3. Third Edition.

Ch 4. Roots of Equations.

Johansson. (2015). Numerical Python: A Practical Techniques Approach for Industry.

Ch. 5. Equation Solving.