Root finding

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Root finding

- Iteration for Solving $x=g(x)$

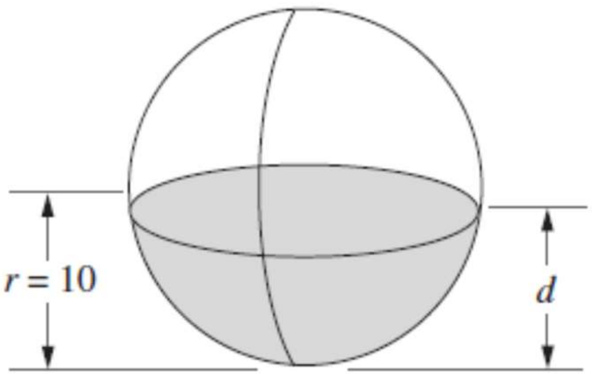
- Bracketing Methods for Locating a Root

- Initial Approximation and Convergence Criteria

- Newton-Raphson and Secant Methods

Solution of nonlinear equations *f*(*x*)=0

An example



$$M_w = \int_0^d \pi(r^2 - (x-r)^2)\,dx = \frac{\pi d^2(3r-d)}{3},$$

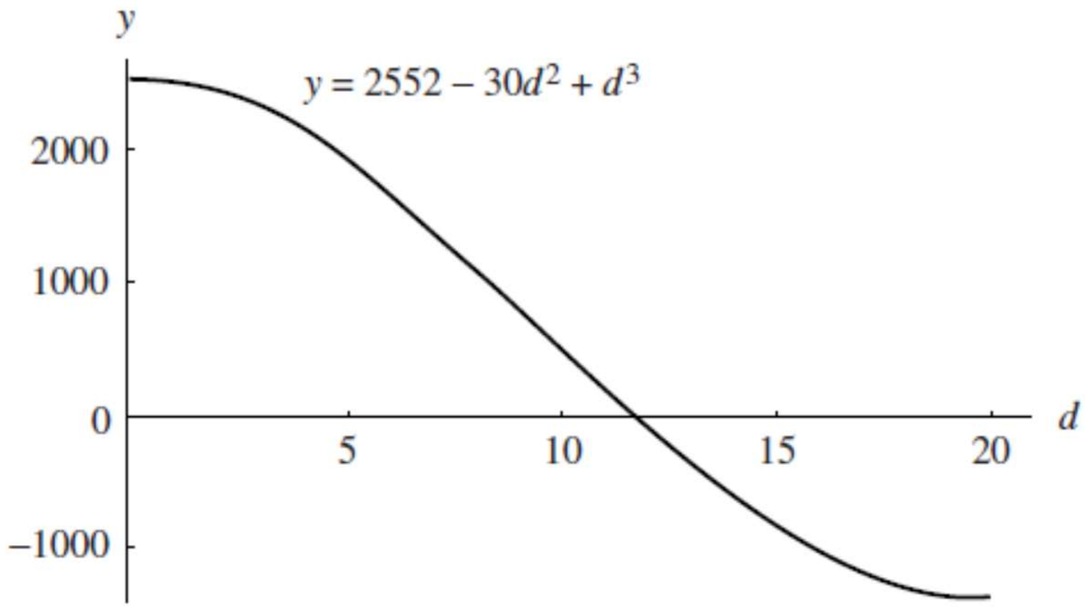
$$M_b = 4\pi r^3 \rho/3.$$

Applying Archimedes' law, $M_w = M_b$,

$$\frac{\pi(d^3 - 3d^2 r + 4r^3\rho)}{3} = 0.$$

An example: r =10 and ρ =0.638

$$\frac{\pi(2552 - 30d^2 + d^3)}{3} = 0. \qquad y = 2552 - 30d^2 + d^3$$



d_1=-8.17607212, d_2=11.86150151, d_3=26.31457061

Iteration for Solving $x=g(x)$

Iteration

$$
\begin{aligned}
&p_0 && \text{(starting value)}\\
p_1 &= g(p_0) &&\\
p_2 &= g(p_1) &&\\
&\vdots &&\\
p_k &= g(p_{k-1}) &&\\
p_{k+1} &= g(p_k) &&\\
&\vdots &&
\end{aligned}
$$

- A sequence of numbers
- If the numbers tend to a limit, $p = g(p)$
- What if the numbers diverge or are periodic?

Divergent iteration

Example 2.1. The iterative rule $p_0 = 1$ and $p_{k+1} = 1.001\,p_k$ for $k = 0, 1, \ldots$ produces a divergent sequence. The first 100 terms look as follows:

$$\begin{aligned}
p_1 &= 1.001\,p_0 &&= (1.001)(1.000000) = 1.001000,\\
p_2 &= 1.001\,p_1 &&= (1.001)(1.001000) = 1.002001,\\
p_3 &= 1.001\,p_2 &&= (1.001)(1.002001) = 1.003003,\\
&\ \vdots && \quad\ \vdots \qquad\qquad\qquad\qquad\quad \vdots\\
p_{100} &= 1.001\,p_{99} &&= (1.001)(1.104012) = 1.105116.
\end{aligned}$$

The process can be continued indefinitely, and it is easily shown that $\lim_{n\to\infty} p_n = +\infty$. In Chapter 9 we will see that the sequence $\{p_k\}$ is a numerical solution to the differential equation $y' = 0.001y$. The solution is known to be $y(x) = e^{0.001x}$. Indeed, if we compare the 100th term in the sequence with $y(100)$, we see that $p_{100} = 1.105116 \approx 1.105171 = e^{0.1} = y(100)$. ■

Finding fixed points

- A **fixed point** of a function $g(x)$ is a real number P such that $P = g(P)$.
- Geometrically, the fixed points of a function $y = g(x)$ are the points of intersection of $y = g(x)$ and $y = x$.
- The iteration $p_{n+1} = g(p_n)$ for $n = 0, 1, \ldots$ is called **fixed-point iteration.**
- Assume that g is a continuous function and that $\{p_n\}$ is a sequence generated by fixed-point iteration. If $\lim_{n \to \infty} p_n = P$, then P is a fixed point of $g(x)$.
- An example

An example

Example 2.2. Consider the convergent iteration

$$p_0 = 0.5 \quad \text{and} \quad p_{k+1} = e^{-p_k} \quad \text{for } k = 0, 1, \ldots.$$

The first 10 terms are obtained by the calculations

$$\begin{aligned}
p_1 &= e^{-0.500000} = 0.606531 \\
p_2 &= e^{-0.606531} = 0.545239 \\
p_3 &= e^{-0.545239} = 0.579703 \\
&\ \ \vdots \qquad\qquad\quad \vdots \\
p_9 &= e^{-0.566409} = 0.567560 \\
p_{10} &= e^{-0.567560} = 0.566907
\end{aligned}$$

The sequence is converging, and further calculations reveal that

$$\lim_{n\to\infty} p_n = 0.567143\ldots.$$

Thus we have found an approximation for the fixed point of the function $y = e^{-x}$.

When does a fixed point exist

Theorem 2.2. Assume that $g \in C[a, b]$.

(3) If the range of the mapping $y = g(x)$ satisfies $y \in [a, b]$ for all $x \in [a, b]$, then g has a fixed point in $[a, b]$.

(4) Furthermore, suppose that $g'(x)$ is defined over (a, b) and that a positive constant $K < 1$ exists with $|g'(x)| \leq K < 1$ for all $x \in (a, b)$; then g has a unique fixed point P in $[a, b]$.

Proof of (3). If $g(a) = a$ or $g(b) = b$, the assertion is true. Otherwise, the values of $g(a)$ and $g(b)$ must satisfy $g(a) \in (a, b]$ and $g(b) \in [a, b)$. The function $f(x) \equiv x - g(x)$ has the property that

$$f(a) = a - g(a) < 0 \quad \text{and} \quad f(b) = b - g(b) > 0.$$

Now apply Theorem 1.2, the intermediate value theorem, to $f(x)$, with the constant $L = 0$, and conclude that there exists a number P with $P \in (a, b)$ so that $f(P) = 0$. Therefore, $P = g(P)$ and P is the desired fixed point of $g(x)$.

Fixed-point theorem

Theorem 2.3 (Fixed-Point Theorem). Assume that (i) $g, g' \in C[a, b]$, (ii) K is a positive constant, (iii) $p_0 \in (a, b)$, and (iv) $g(x) \in [a, b]$ for all $x \in [a, b]$.

(6) If $|g'(x)| \leq K < 1$ for all $x \in [a, b]$, then the iteration $p_n = g(p_{n-1})$ will converge to the unique fixed point $P \in [a, b]$. In this case, P is said to be an attractive fixed point.

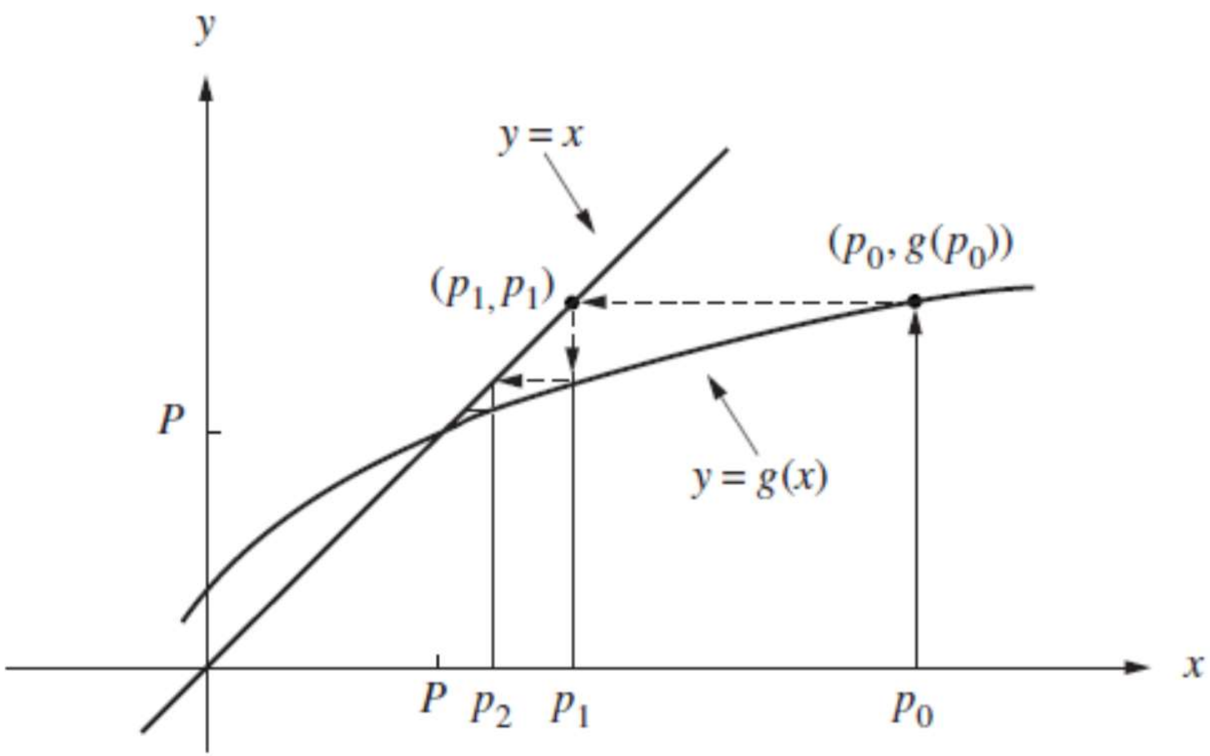


Figure 2.4 (a) Monotone convergence when $0 < g'(P) < 1$.

Fixed-point theorem

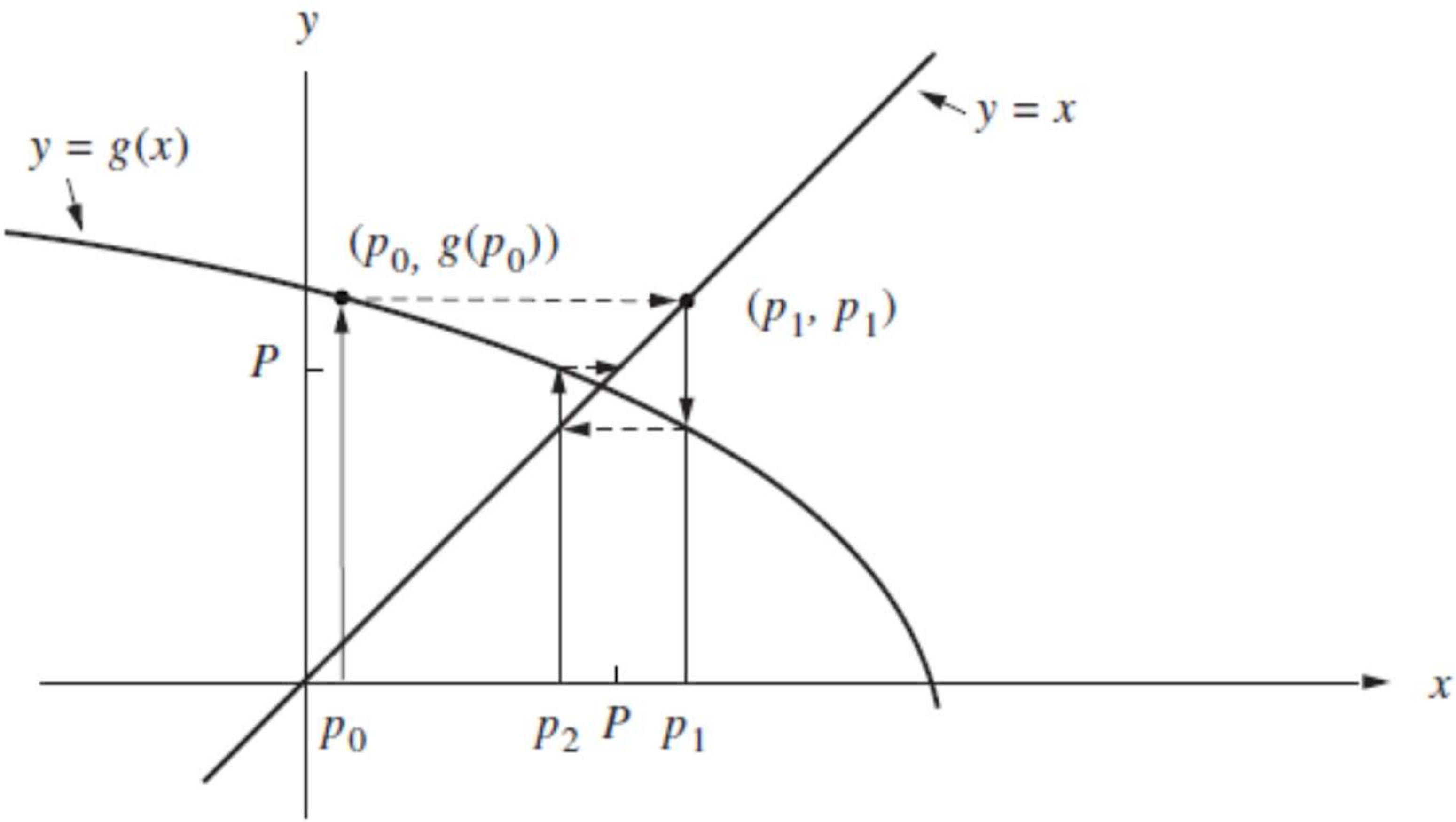


Figure 2.4 (b) Oscillating convergence when $-1 < g'(P) < 0$.

Fixed-point theorem

Theorem 2.3 (Fixed-Point Theorem). Assume that (i) $g, g' \in C[a, b]$, (ii) K is a positive constant, (iii) $p_0 \in (a, b)$, and (iv) $g(x) \in [a, b]$ for all $x \in [a, b]$.

(7) If $|g'(x)| > 1$ for all $x \in [a, b]$, then the iteration $p_n = g(p_{n-1})$ will not converge to P. In this case, P is said to be a repelling fixed point and the iteration exhibits local divergence.

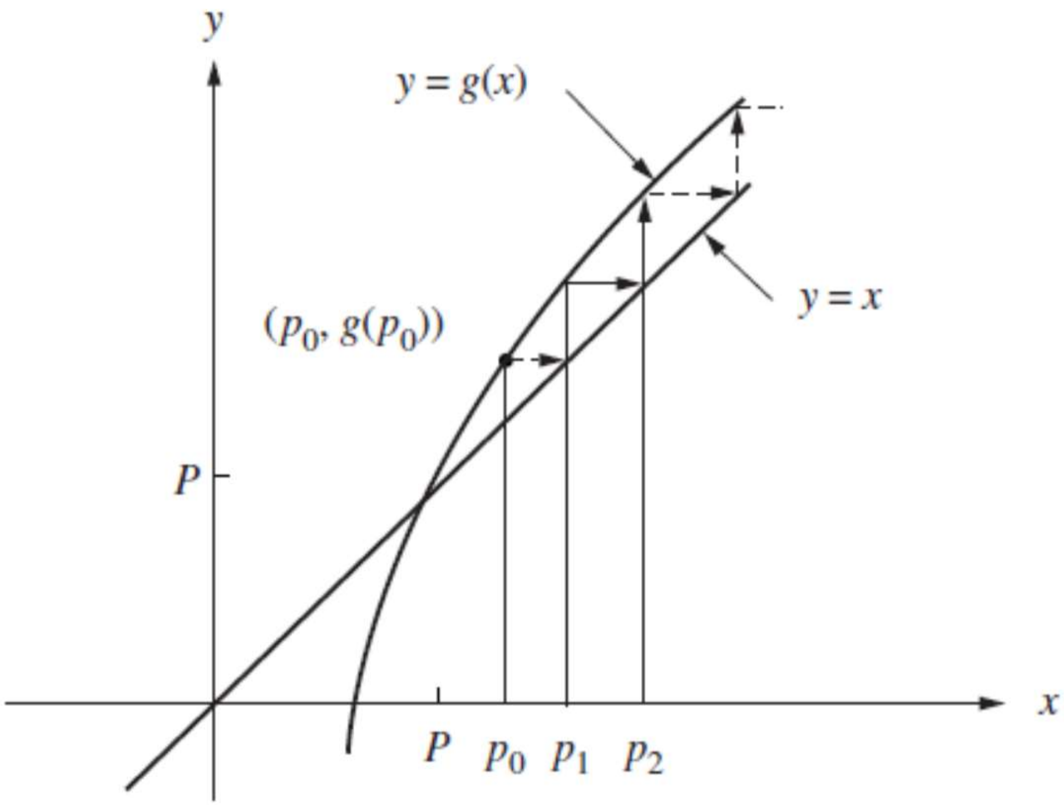


Figure 2.5 (a) Monotone divergence when $1 < g'(P)$.

Fixed-point theorem

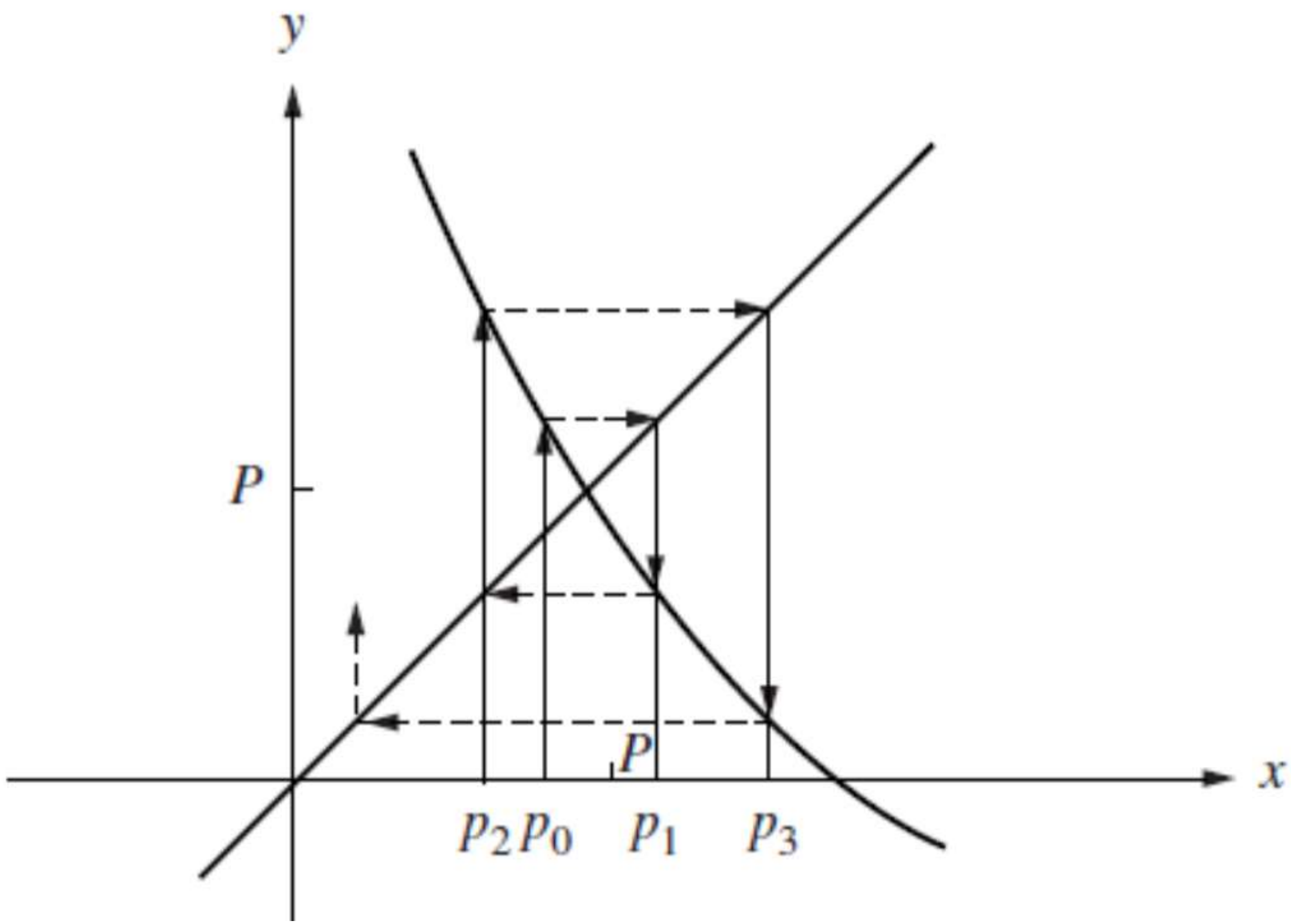


Figure 2.5 (b) Divergent oscillation when $g'(P) < -1$.

An example

Example 2.4. Consider the iteration $p_{n+1} = g(p_n)$ when the function $g(x) = 1+x-x^2/4$ is used. The fixed points can be found by solving the equation $x = g(x)$. The two solutions (fixed points of g) are $x = -2$ and $x = 2$. The derivative of the function is $g'(x) = 1-x/2$, and there are only two cases to consider.

Case (i): $P = -2$

Start with $p_0 = -2.05$

then get

$$p_1 = -2.100625$$
$$p_2 = -2.20378135$$
$$p_3 = -2.41794441$$
$$\vdots$$
$$\lim_{n\to\infty} p_n = -\infty.$$

Since $|g'(x)| > \frac{3}{2}$ on $[-3, -1]$, by Theorem 2.3, the sequence will not converge to $P = -2$.

Case (ii): $P = 2$

Start with $p_0 = 1.6$

then get

$$p_1 = 1.96$$
$$p_2 = 1.9996$$
$$p_3 = 1.99999996$$
$$\vdots$$
$$\lim_{n\to\infty} p_n = 2.$$

Since $|g'(x)| < \frac{1}{2}$ on $[1, 3]$, by Theorem 2.3, the sequence will converge to $P = 2$.

■

What will happen when $g`(P)=1$?

Another example

Example 2.5. Consider the iteration $p_{n+1} = g(p_n)$ when the function $g(x) = 2(x-1)^{1/2}$ for $x \geq 1$ is used. Only one fixed point $P = 2$ exists. The derivative is $g'(x) = 1/(x-1)^{1/2}$ and $g'(2) = 1$, so Theorem 2.3 does not apply. There are two cases to consider when the starting value lies to the left or right of $P = 2$.

Case (i): Start with $p_0 = 1.5$,

then get
$$\begin{aligned} p_1 &= 1.41421356 \\ p_2 &= 1.28718851 \\ p_3 &= 1.07179943 \\ p_4 &= 0.53590832 \\ &\vdots \\ p_5 &= 2(-0.46409168)^{1/2}. \end{aligned}$$

Since p_4 lies outside the domain of $g(x)$, the term p_5 cannot be computed.

Case (ii): Start with $p_0 = 2.5$,

then get
$$\begin{aligned} p_1 &= 2.44948974 \\ p_2 &= 2.40789513 \\ p_3 &= 2.37309514 \\ p_4 &= 2.34358284 \\ &\vdots \\ \lim_{n\to\infty} p_n &= 2. \end{aligned}$$

This sequence is converging too slowly to the value $P = 2$; indeed, $P_{1000} = 2.00398714$.

Absolute and relative error consideration

- In last example, case (ii), the sequence converges slowly, and after 1000 iterations

$$p_{1000} = 2.00398714, \quad p_{1001} = 2.00398317, \quad \text{and} \quad p_{1002} = 2.00397921.$$

- Probably find convergence after a few thousand more iterations.
- What about a criterion for stopping the iteration?

- Relative error:

$$|p_{1001} - p_{1002}| = |2.00398317 - 2.00397921| = 0.00000396.$$

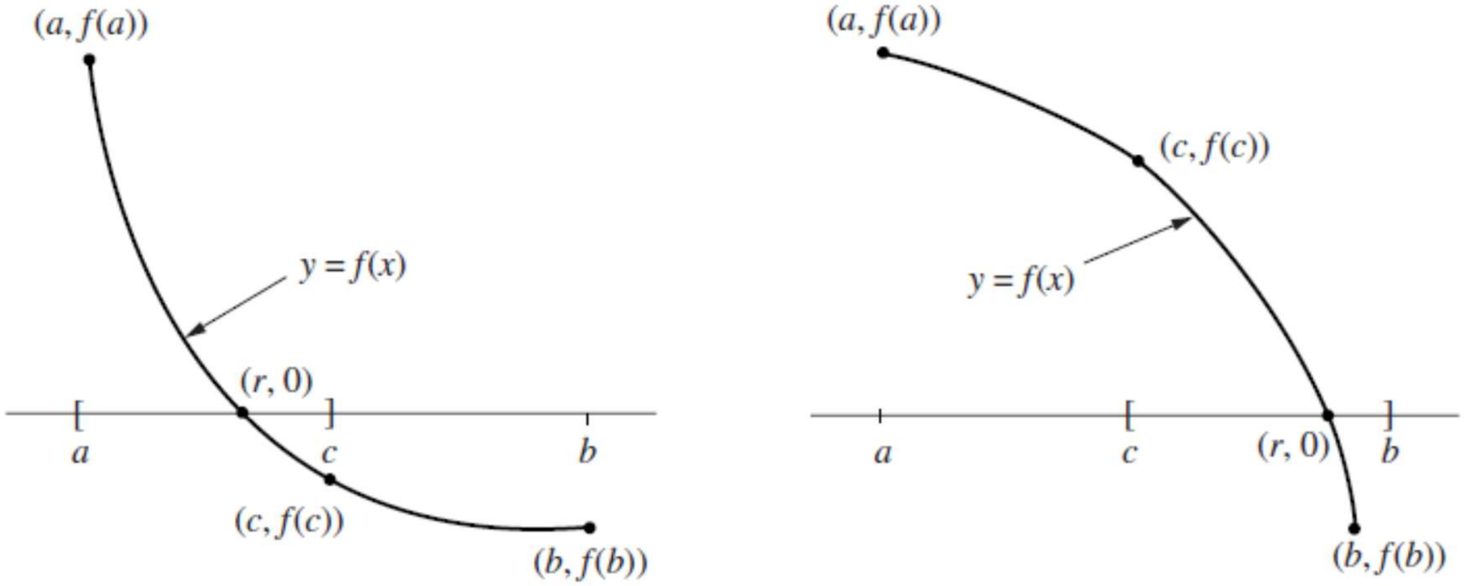
- Absolute error:

$$|P - p_{1000}| = |2.00000000 - 2.00398714| = 0.00398714.$$

Bracketing Methods for Locating a Root

Bisection method of Bolzano

- Consider a function $f(x)$ which is continuous at interval $[a, b]$, and $f(a)$ and $f(b)$ have opposite signs
- The bisection method systematically moves the endpoints of the interval closer and closer together until we obtain an interval of arbitrarily small width that brackets the zero.



(a) If $f(a)$ and $f(c)$ have opposite signs, then squeeze from the right.

(b) If $f(c)$ and $f(b)$ have opposite signs, then squeeze from the left.

Bisection theorem

$$(8) \qquad a_0 \le a_1 \le \cdots \le a_n \le \cdots \le r \le \cdots \le b_n \le \cdots \le b_1 \le b_0,$$

where $c_n = (a_n + b_n)/2$, and if $f(a_{n+1})f(b_{n+1}) < 0$, then

$$(9) \qquad [a_{n+1}, b_{n+1}] = [a_n, c_n] \quad \text{or} \quad [a_{n+1}, b_{n+1}] = [c_n, b_n] \quad \text{for all } n.$$

Theorem 2.4 (Bisection Theorem). Assume that $f \in C[a,b]$ and that there exists a number $r \in [a,b]$ such that $f(r) = 0$. If $f(a)$ and $f(b)$ have opposite signs, and $\{c_n\}_{n=0}^{\infty}$ represents the sequence of midpoints generated by the bisection process of (8) and (9), then

$$(10) \qquad |r - c_n| \le \frac{b-a}{2^{n+1}} \quad \text{for } n = 0, 1, \ldots,$$

and therefore the sequence $\{c_n\}_{n=0}^{\infty}$ converges to the zero $x = r$; that is,

$$(11) \qquad \lim_{n \to \infty} c_n = r.$$

An example

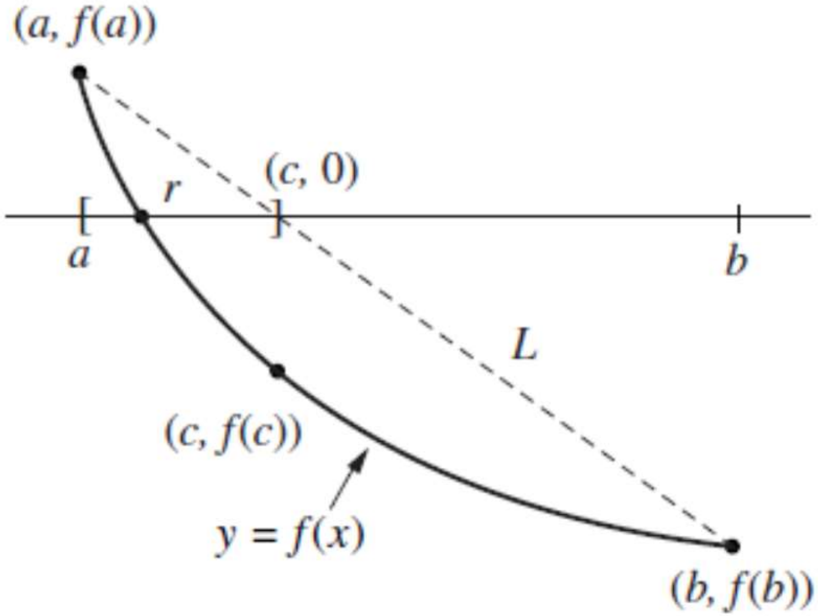
Table 2.1 Bisection Method Solution of $x\sin(x) - 1 = 0$

k	Left endpoint, a_k	Midpoint, c_k	Right endpoint, b_k	Function value, $f(c_k)$
0	0	1.	2.	−0.158529
1	1.0	1.5	2.0	0.496242
2	1.00	1.25	1.50	0.186231
3	1.000	1.125	1.250	0.015051
4	1.0000	1.0625	1.1250	−0.071827
5	1.06250	1.09375	1.12500	−0.028362
6	1.093750	1.109375	1.125000	−0.006643
7	1.1093750	1.1171875	1.1250000	0.004208
8	1.10937500	1.11328125	1.11718750	−0.001216
⋮	⋮	⋮	⋮	⋮

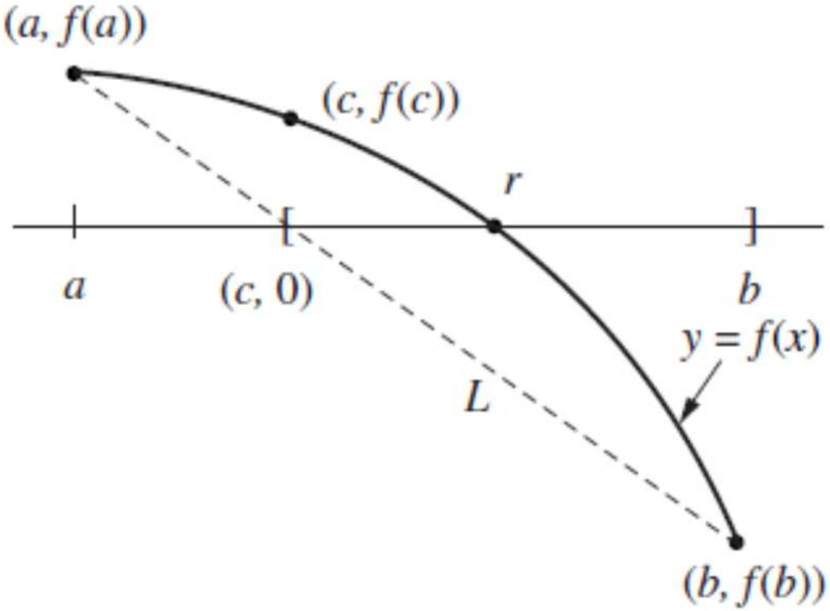
Converges to r = 1.114157141…

Method of false position

- Converges much faster



(a) If $f(a)$ and $f(c)$ have opposite signs, then squeeze from the right.



(b) If $f(c)$ and $f(b)$ have opposite signs, then squeeze from the left.

Convergence of the False Position Method

$$c_n = b_n - \frac{f(b_n)(b_n - a_n)}{f(b_n) - f(a_n)},$$

- the sequence c_n will converge to r .
- But beware; although the interval width $b_n - a_n$ is getting smaller, it is possible that it may not go to zero.

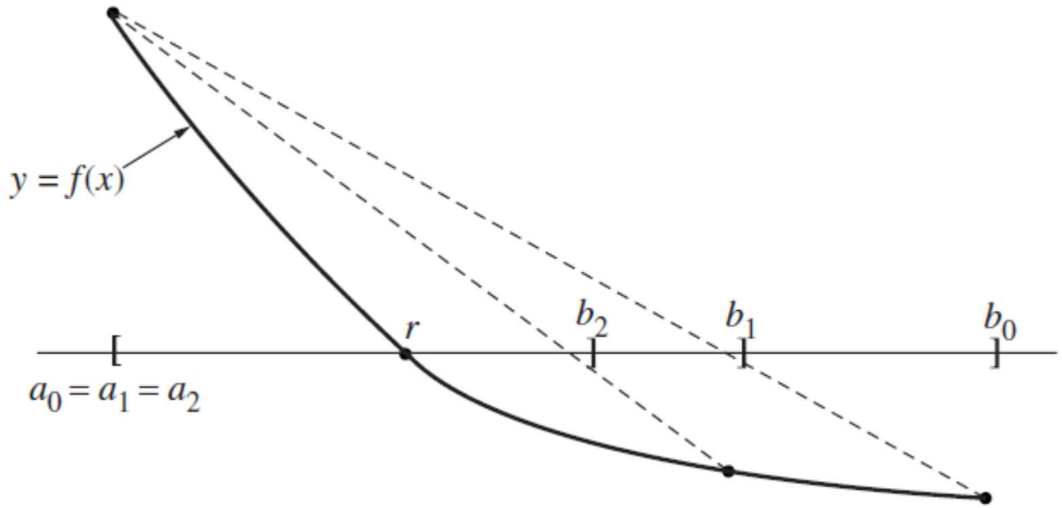


Figure 2.9 The stationary endpoint for the false position method.

An example

Table 2.2 False Position Method Solution of $x \sin(x) - 1 = 0$

k	Left endpoint, a_k	Midpoint, c_k	Right endpoint, b_k	Function value, $f(c_k)$
0	0.00000000	1.09975017	2.00000000	−0.02001921
1	1.09975017	1.12124074	2.00000000	0.00983461
2	1.09975017	1.11416120	1.12124074	0.00000563
3	1.09975017	1.11415714	1.11416120	0.00000000

Converges to r = 1.11415714 much faster

The termination criterion is different

Initial Approximation and Convergence Criteria

Initial Approximation and Convergence Criteria

- **Bracketing methods: globally convergent**. Once the interval has been found, the iterations will proceed until a root is found
- **Newton-Raphson method or secant method: locally convergent.** Require that a close approximation to the root; converge more rapidly.
- View the graph $y = f(x)$ and make decisions based on what it looks like.

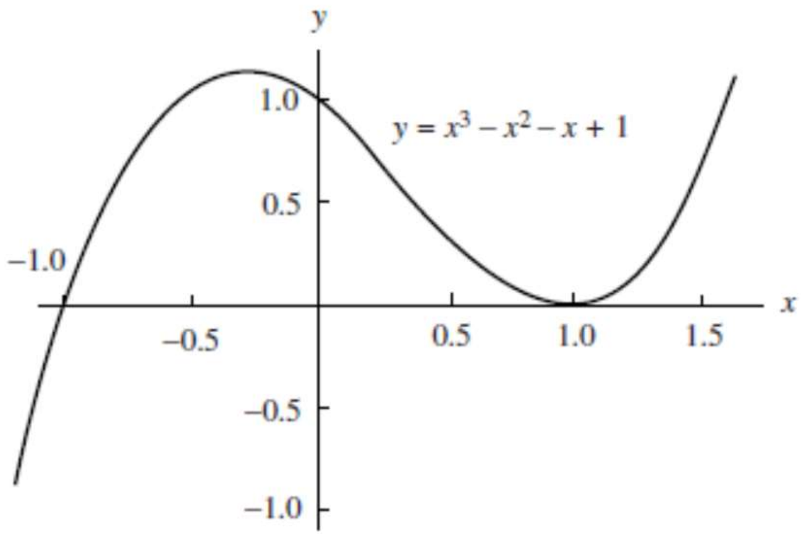


Figure 2.10 The graph of the cubic polynomial $y = x^3 - x^2 - x + 1$.

Checking for convergence

- An algorithm must be used to compute a value p_n that is an acceptable computer solution

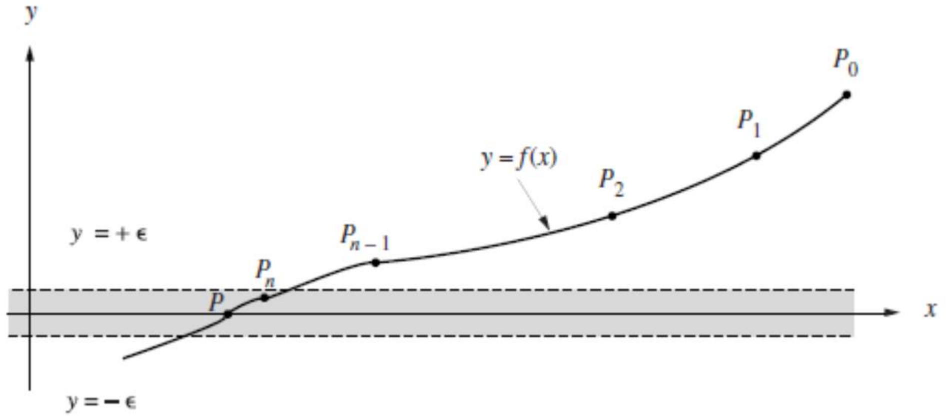


Figure 2.11 (a) The horizontal convergence band for locating a solution to $f(x) = 0$.

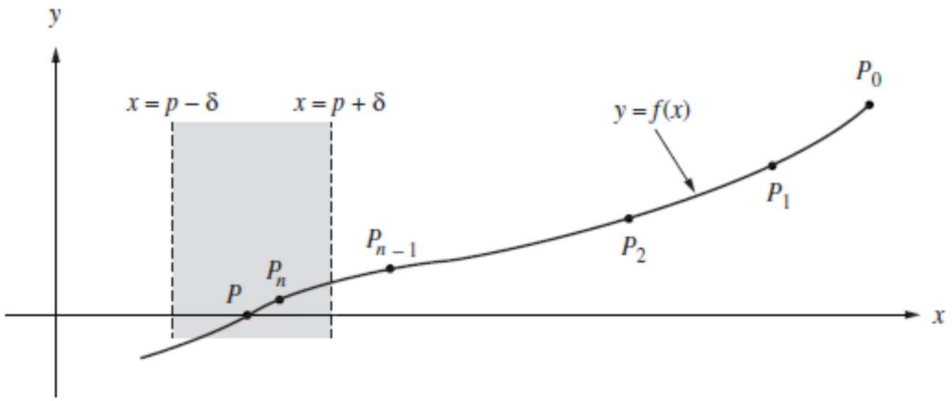


Figure 2.11 (b) The vertical convergence band for locating a solution to $f(x) = 0$.

Checking for convergence

- The second criterion is often desired, but it is difficult to implement because it involves the unknown solution *p*. Instead $p_n \approx p_{n-1}$ can be used.

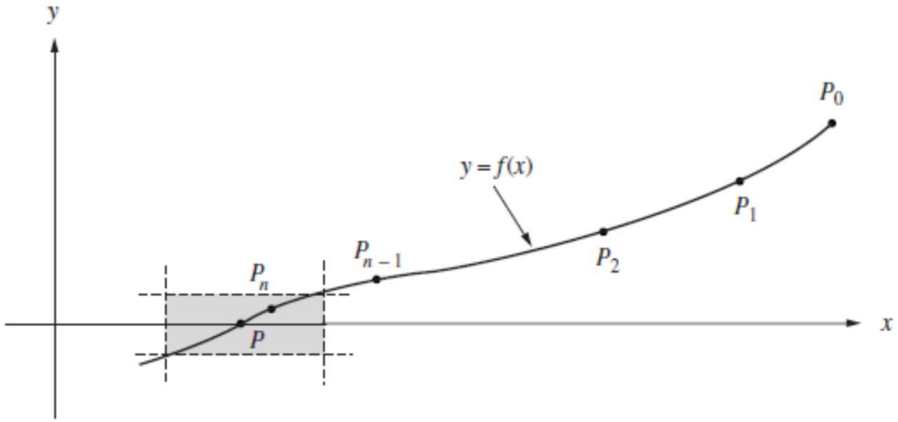


Figure 2.12 (a) The rectangular region defined by $|x - p| < \delta$ AND $|y| < \epsilon$.

The size of the tolerances δ and ε are crucial

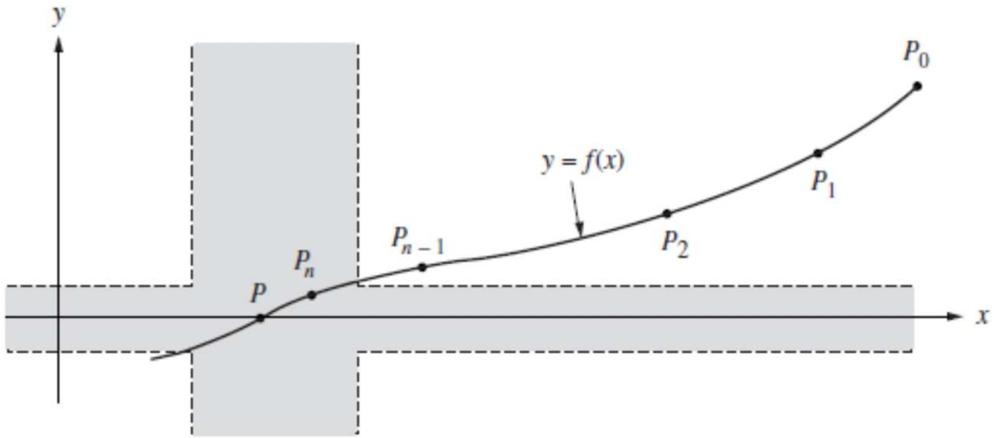
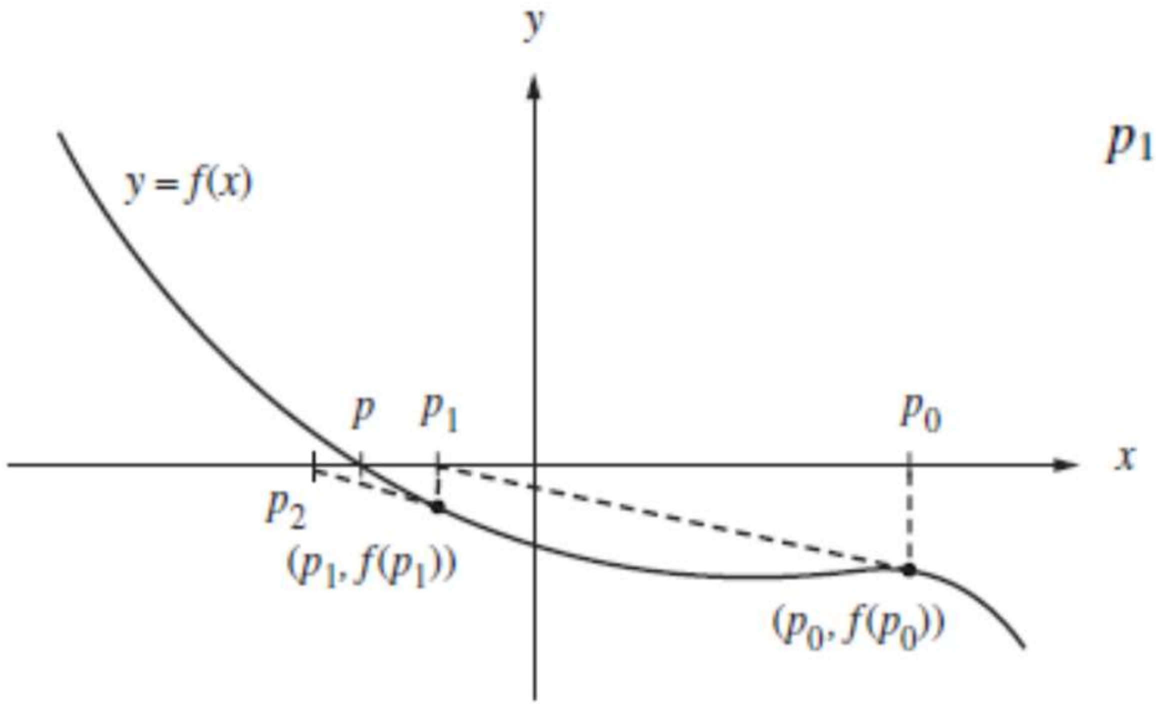


Figure 2.12 (b) The unbounded region defined by $|x - p| < \delta$ OR $|y| < \epsilon$.

Newton-Raphson and Secant Methods

Slope Methods for Finding Roots

- If $f(x)$, $f^{`}(x)$, and $f^{``}(x)$ are continuous near a root p, then this extra information regarding the nature of $f(x)$ can be used to develop algorithms that will produce sequences $\{p_k\}$ that converge faster to p than either the bisection or false position method.



$$p_1 = p_0 - \frac{f(p_0)}{f'(p_0)}.$$

Figure 2.13 The geometric construction of p_1 and p_2 for the Newton-Raphson method.

Newton-Raphson Theorem

Theorem 2.5 (Newton-Raphson Theorem). Assume that $f \in C^2[a, b]$ and there exists a number $p \in [a, b]$, where $f(p) = 0$. If $f'(p) \neq 0$, then there exists a $\delta > 0$ such that the sequence $\{p_k\}_{k=0}^{\infty}$ defined by the iteration

$$p_k = g(p_{k-1}) = p_{k-1} - \frac{f(p_{k-1})}{f'(p_{k-1})} \quad \text{for } k = 1, 2, \ldots \tag{4}$$

will converge to p for any initial approximation $p_0 \in [p - \delta, p + \delta]$.

Remark. The function $g(x)$ defined by the formula

$$g(x) = x - \frac{f(x)}{f'(x)} \tag{5}$$

is called the ***Newton-Raphson iteration function***. Since $f(p) = 0$, it is easy to see that $g(p) = p$. Thus the Newton-Raphson iteration for finding the root of the equation $f(x) = 0$ is accomplished by finding a fixed point of the function $g(x)$.

Newton's Iteration for Finding Square Roots

Corollary 2.2 **(Newton's Iteration for Finding Square Roots).** Assume that $A > 0$ is a real number and let $p_0 > 0$ be an initial approximation to $\sqrt{A}$. Define the sequence $\{p_k\}_{k=0}^{\infty}$ using the recursive rule

$$(11) \qquad p_k = \frac{p_{k-1} + \dfrac{A}{p_{k-1}}}{2} \quad \text{for } k = 1,\ 2,\ \ldots.$$

Then the sequence $\{p_k\}_{k=0}^{\infty}$ converges to $\sqrt{A}$; that is, $\lim_{n\to\infty} p_k = \sqrt{A}$.

Outline of Proof. Start with the function $f(x) = x^2 - A$, and notice that the roots of the equation $x^2 - A = 0$ are $\pm\sqrt{A}$. Now use $f(x)$ and the derivative $f'(x)$ in formula (5) and write down the Newton-Raphson iteration formula

$$(12) \qquad g(x) = x - \frac{f(x)}{f'(x)} = x - \frac{x^2 - A}{2x}.$$

This formula can be simplified to obtain

$$(13) \qquad g(x) = \frac{x + \dfrac{A}{x}}{2}.$$

When $g(x)$ in (13) is used to define the recursive iteration in (4), the result is formula (11). It can be proved that the sequence that is generated in (11) will converge for any starting value $p_0 > 0$. The details are left for the exercises. •

An example

Example 2.11. Use Newton's square-root algorithm to find $\sqrt{5}$.

Starting with $p_0 = 2$ and using formula (11), we compute

$$\begin{aligned}
p_1 &= \frac{2 + 5/2}{2} = 2.25 \\
p_2 &= \frac{2.25 + 5/2.25}{2} = 2.236111111 \\
p_3 &= \frac{2.236111111 + 5/2.236111111}{2} = 2.236067978 \\
p_4 &= \frac{2.36067978 + 5/2.236067978}{2} = 2.236067978.
\end{aligned}$$

Further iterations produce $p_k \approx 2.236067978$ for $k > 4$, so we see that convergence accurate to nine decimal places has been achieved. ■

A real example: a fired projectile

Ideal model $y = v_y t - 16t^2$ and $x = v_x t,$

More realistic model $y = f(t) = (Cv_y + 32C^2)\left(1 - e^{-t/C}\right) - 32Ct$

$$x = r(t) = Cv_x\left(1 - e^{-t/C}\right),$$

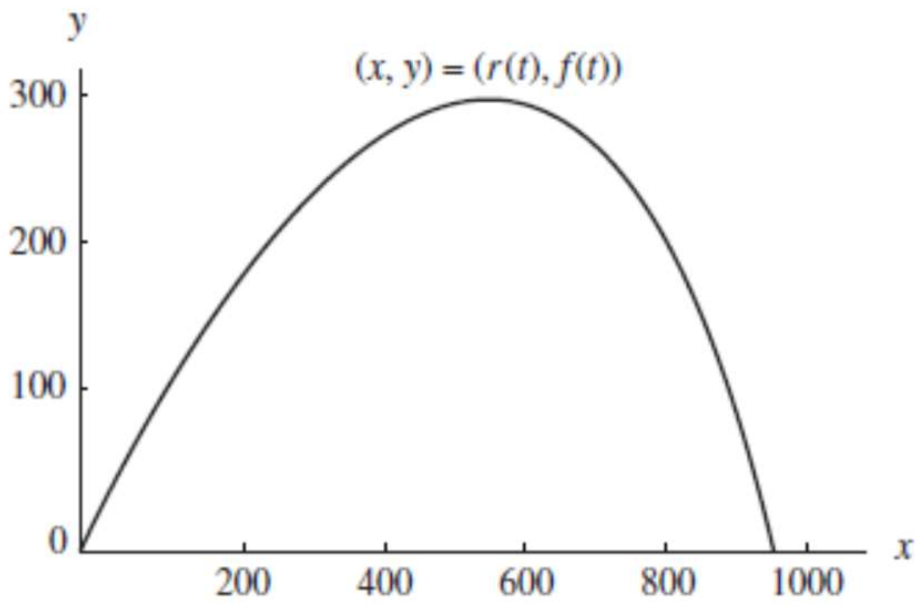


Figure 2.14 The path of a projectile with air resistance considered.

A real example: a fired projectile

Example 2.12. A projectile is fired with an angle of elevation $b_0 = 45°$, $v_y = v_x = 160$ ft/sec, and $C = 10$. Find the elapsed time until impact and find the range.

Using formulas (15) and (16), the equations of motion are $y = f(t) = 4800(1 - e^{-t/10}) - 320t$ and $x = r(t) = 1600(1 - e^{-t/10})$. Since $f(8) = 83.220972$ and $f(9) = -31.534367$, we will use the initial guess $p_0 = 8$. The derivative is $f'(t) = 480e^{-t/10} - 320$, and its value $f'(p_0) = f'(8) = -104.3220972$ is used in formula (4) to get

$$p_1 = 8 - \frac{83.22097200}{-104.3220972} = 8.797731010.$$

A summary of the calculation is given in Table 2.4.

The value p_4 has eight decimal places of accuracy, and the time until impact is $t \approx 8.74217466$ seconds. The range can now be computed using $r(t)$, and we get

$$r(8.74217466) = 1600\left(1 - e^{-0.874217466}\right) = 932.4986302 \text{ ft.} \qquad \blacksquare$$

Table 2.4 Finding the Time When the Height $f(t)$ Is Zero

k	Time, p_k	$p_{k+1} - p_k$	Height, $f(p_k)$
0	8.00000000	0.79773101	83.22097200
1	8.79773101	−0.05530160	−6.68369700
2	8.74242941	−0.00025475	−0.03050700
3	8.74217467	−0.00000001	−0.00000100
4	8.74217466	0.00000000	0.00000000

Speed of Convergence

- Simple root or multiple root

Definition 2.4. Assume that $f(x)$ and its derivatives $f'(x), \ldots, f^{(M)}(x)$ are defined and continuous on an interval about $x = p$. We say that $f(x) = 0$ has a ***root of order M*** at $x = p$ if and only if

$$(17)\quad f(p) = 0, \qquad f'(p) = 0, \qquad \ldots, \qquad f^{(M-1)}(p) = 0, \qquad \text{and} \qquad f^{(M)}(p) \neq 0.$$

A root of order $M = 1$ is often called a *simple root*, and if $M > 1$, it is called a *multiple root*. A root of order $M = 2$ is sometimes called a *double root*, and so on. The next result will illuminate these concepts. ▲

Lemma 2.1. If the equation $f(x) = 0$ has a root of order M at $x = p$, then there exists a continuous function $h(x)$ so that $f(x)$ can be expressed as the product

$$(18)\qquad f(x) = (x - p)^M h(x), \qquad \text{where } h(p) \neq 0.$$

Example 2.13. The function $f(x) = x^3 - 3x + 2$ has a simple root at $p = -2$ and a double root at $p = 1$. This can be verified by considering the derivatives $f'(x) = 3x^2 - 3$ and $f''(x) = 6x$. At the value $p = -2$, we have $f(-2) = 0$ and $f'(-2) = 9$, so $M = 1$ in Definition 2.4; hence $p = -2$ is a simple root. For the value $p = 1$, we have $f(1) = 0$, $f'(1) = 0$, and $f''(1) = 6$, so $M = 2$ in Definition 2.4; hence $p = 1$ is a double root. Also, notice that $f(x)$ has the factorization $f(x) = (x + 2)(x - 1)^2$. ■

Speed of Convergence

- Order of convergence

Definition 2.5. Assume that $\{p_n\}_{n=0}^{\infty}$ converges to p and set $E_n = p - p_n$ for $n \geq 0$. If two positive constants $A \neq 0$ and $R > 0$ exist, and

$$\lim_{n\to\infty} \frac{|p - p_{n+1}|}{|p - p_n|^R} = \lim_{n\to\infty} \frac{|E_{n+1}|}{|E_n|^R} = A, \tag{19}$$

then the sequence is said to converge to p with ***order of convergence*** R. The number A is called the *asymptotic error constant*. The cases $R = 1, 2$ are given special consideration.

(20) If $R = 1$, the convergence of $\{p_n\}_{n=0}^{\infty}$ is called ***linear***.
If $R = 2$, the convergence of $\{p_n\}_{n=0}^{\infty}$ is called ***quadratic***. ▲

- If R is large, converges more rapidly

- Some sequences converge at a rate that is not an integer. For example, the order of convergence of the secant method is $R \approx 1.618$

Example: Quadratic convergence

Example 2.14 (Quadratic Convergence at a Simple Root). Start with $p_0 = -2.4$ and use Newton-Raphson iteration to find the root $p = -2$ of the polynomial $f(x) = x^3 - 3x + 2$. The iteration formula for computing $\{p_k\}$ is

$$p_k = g(p_{k-1}) = \frac{2p_{k-1}^3 - 2}{3p_{k-1}^2 - 3}. \tag{21}$$

Table 2.5 Newton's Method Converges Quadratically at a Simple Root

k	p_k	$p_{k+1} - p_k$	$E_k = p - p_k$	$\frac{\lvert E_{k+1}\rvert}{\lvert E_k\rvert^2}$
0	−2.400000000	0.323809524	0.400000000	0.476190475
1	−2.076190476	0.072594465	0.076190476	0.619469086
2	−2.003596011	0.003587422	0.003596011	0.664202613
3	−2.000008589	0.000008589	0.000008589	
4	−2.000000000	0.000000000	0.000000000	

Example: Linear convergence

Example 2.15 (Linear Convergence at a Double Root). Start with $p_0 = 1.2$ and use Newton-Raphson iteration to find the double root $p = 1$ of the polynomial $f(x) = x^3 - 3x + 2$. Using formula (20) to check for linear convergence, we get the values in Table 2.6.

Table 2.6 Newton's Method Converges Linearly at a Double Root

k	p_k	$p_{k+1} - p_k$	$E_k = p - p_k$	$\frac{\lvert E_{k+1}\rvert}{\lvert E_k\rvert}$
0	1.200000000	−0.096969697	−0.200000000	0.515151515
1	1.103030303	−0.050673883	−0.103030303	0.508165253
2	1.052356420	−0.025955609	−0.052356420	0.496751115
3	1.026400811	−0.013143081	−0.026400811	0.509753688
4	1.013257730	−0.006614311	−0.013257730	0.501097775
5	1.006643419	−0.003318055	−0.006643419	0.500550093
⋮	⋮	⋮	⋮	⋮

Pitfalls

- Sometimes the initial approximation p_0 is too far away from the desired root and the sequence $\{p_k\}$ converges to some other root

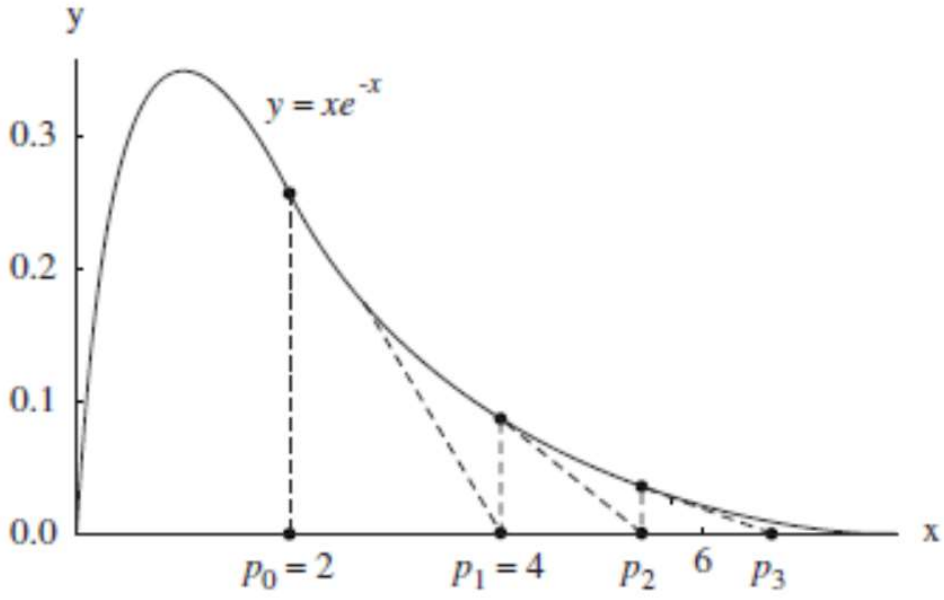


Figure 2.15 (a) Newton-Raphson iteration for $f(x) = xe^{-x}$ can produce a divergent sequence.

- This particular function has another surprising problem. The value of $f(x)$ goes to zero rapidly as x gets large, for example, $f(p_{15}) = 0.0000000536$, and it is possible that p_{15} could be mistaken for a root.

Pitfalls

- **Cycling**, occurs when the terms in the sequence $\{p_k\}$ tend to repeat or almost repeat.

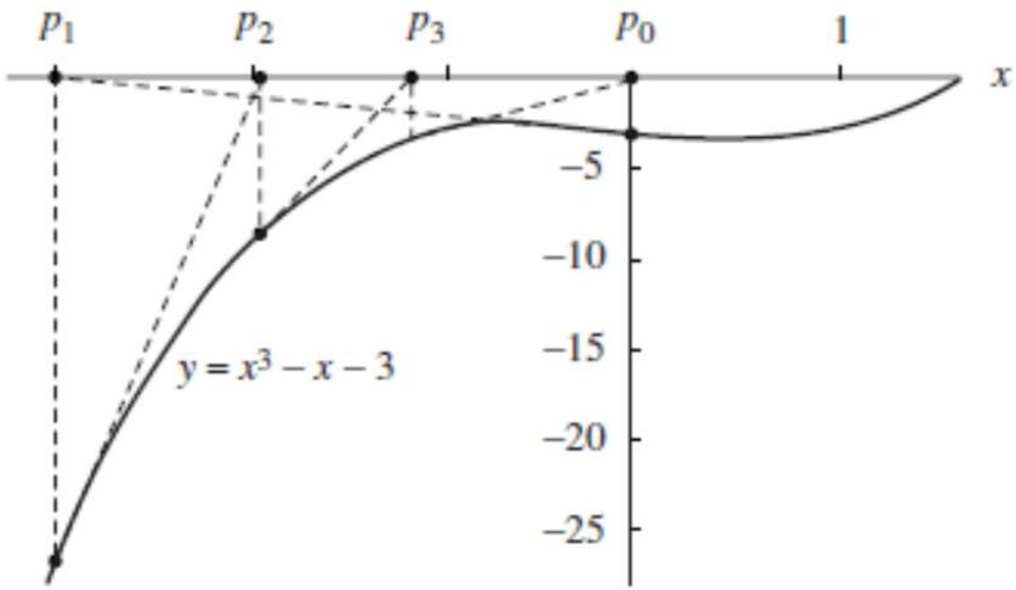


Figure 2.15 (b) Newton-Raphson iteration for $f(x) = x^3 - x - 3$ can produce a cyclic sequence.

- Chosen P_0=0, stuck in a cycle

- Chosen P_0=2, the sequence converges

Pitfalls

- **Divergent oscillation**, occurs when $|g'(x)| \geq 1$ on an interval containing the root p

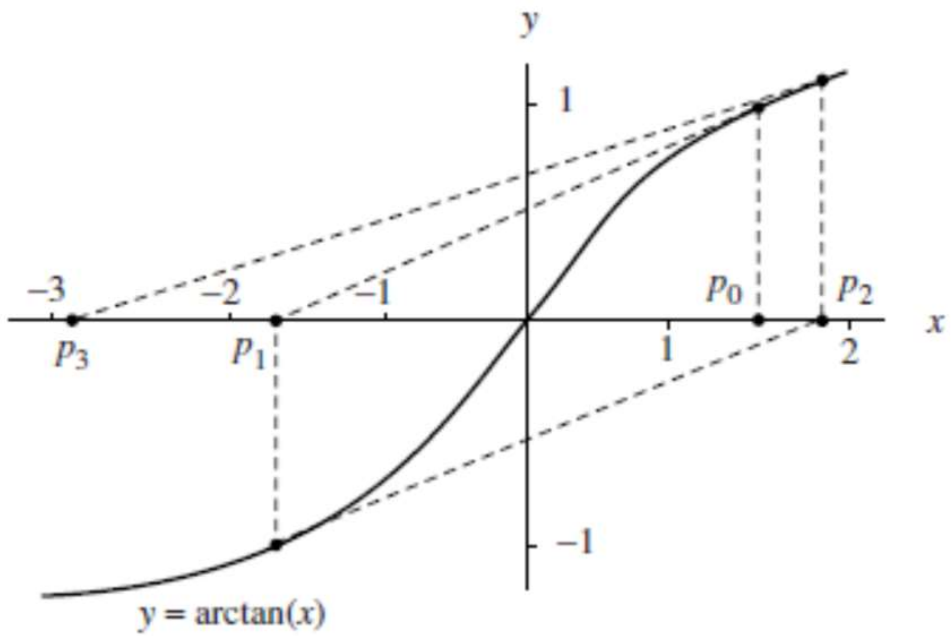


Figure 2.15 (c) Newton-Raphson iteration for $f(x) = \arctan(x)$ can produce a divergent oscillating sequence.

- But if the starting value is sufficiently close to the root $p = 0$, a convergent sequence results

Secant Method

- The Newton-Raphson algorithm requires the evaluation of two functions per iteration, $f(p_{k-1})$ and $f`(p_{k-1})$

- Many functions have nonelementary forms (integrals, sums, etc.), and it is desirable to have a method that converges almost as fast as Newton's method yet involves only evaluations of $f(x)$ and not of $f`(x)$.

- The secant method will require only one evaluation of $f(x)$ per step and at a simple root has an order of convergence $R \approx 1.618033989$. It is almost as fast as Newton's method, which has order 2.

- The formula involved in the secant method is the same one that was used in the regula falsi method, except that the logical decisions regarding how to define each succeeding term are different.

Secant Method

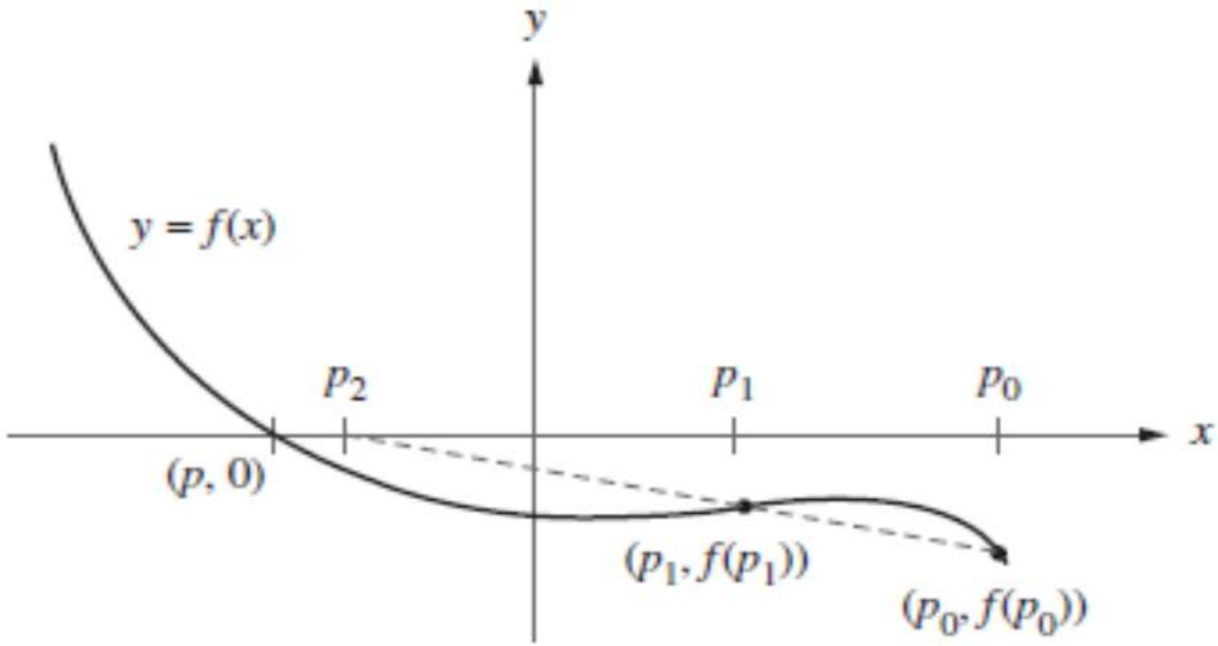


Figure 2.16 The geometric construction of p_2 for the secant method.

$$p_2 = g(p_1, p_0) = p_1 - \frac{f(p_1)(p_1 - p_0)}{f(p_1) - f(p_0)}. \tag{25}$$

The general term is given by the two-point iteration formula

$$p_{k+1} = g(p_k, p_{k-1}) = p_k - \frac{f(p_k)(p_k - p_{k-1})}{f(p_k) - f(p_{k-1})}. \tag{26}$$

Secant Method: An example

Example 2.16 (Secant Method at a Simple Root). Start with $p_0 = -2.6$ and $p_1 = -2.4$ and use the secant method to find the root $p = -2$ of the polynomial function $f(x) = x^3 - 3x + 2$.

In this case the iteration formula (27) is

$$p_{k+1} = g(p_k, p_{k-1}) = p_k - \frac{(p_k^3 - 3p_k + 2)(p_k - p_{k-1})}{p_k^3 - p_{k-1}^3 - 3p_k + 3p_{k-1}}. \tag{27}$$

This can be algebraically manipulated to obtain

$$p_{k+1} = g(p_k, p_{k-1}) = \frac{p_k^2 p_{k-1} + p_k p_{k-1}^2 - 2}{p_k^2 + p_k p_{k-1} + p_{k-1}^2 - 3}. \tag{28}$$

Table 2.7 Convergence of the Secant Method at a Simple Root

k	p_k	$p_{k+1} - p_k$	$E_k = p - p_k$	$\frac{\|E_{k+1}\|}{\|E_k\|^{1.618}}$
0	−2.600000000	0.200000000	0.600000000	0.914152831
1	−2.400000000	0.293401015	0.400000000	0.469497765
2	−2.106598985	0.083957573	0.106598985	0.847290012
3	−2.022641412	0.021130314	0.022641412	0.693608922
4	−2.001511098	0.001488561	0.001511098	0.825841116
5	−2.000022537	0.000022515	0.000022537	0.727100987
6	−2.000000022	0.000000022	0.000000022	
7	−2.000000000	0.000000000	0.000000000	

Accelerated Convergence

Theorem 2.7 (Acceleration of Newton-Raphson Iteration). Suppose that the Newton-Raphson algorithm produces a sequence that converges linearly to the root $x = p$ of order $M > 1$. Then the Newton-Raphson iteration formula

$$p_k = p_{k-1} - \frac{Mf(p_{k-1})}{f'(p_{k-1})} \tag{30}$$

will produce a sequence $\{p_k\}_{k=0}^{\infty}$ that converges quadratically to p.

Example 2.17 (Acceleration of Convergence at a Double Root). Start with $p_0 = 1.2$ and use accelerated Newton-Raphson iteration to find the double root $p = 1$ of $f(x) = x^3 - 3x + 2$.

Since $M = 2$, the acceleration formula (31) becomes

$$p_k = p_{k-1} - 2\frac{f(p_{k-1})}{f'(p_{k-1})} = \frac{p_{k-1}^3 + 3p_{k-1} - 4}{3p_{k-1}^2 - 3},$$

k	p_k	$p_{k+1} - p_k$	$E_k = p - p_k$	$\frac{\lvert E_{k+1}\rvert}{\lvert E_k\rvert^2}$
0	1.200000000	−0.193939394	−0.200000000	0.151515150
1	1.006060606	−0.006054519	−0.006060606	0.165718578
2	1.000006087	−0.000006087	−0.000006087	
3	1.000000000	0.000000000	0.000000000	

Comparison of the Speed of Convergence

Method	Special considerations	Relation between successive error terms
Bisection		$E_{k+1} \approx \frac{1}{2}\lvert E_k \rvert$
Regula falsi		$E_{k+1} \approx A\lvert E_k \rvert$
Secant method	Multiple root	$E_{k+1} \approx A\lvert E_k \rvert$
Newton-Raphson	Multiple root	$E_{k+1} \approx A\lvert E_k \rvert$
Secant method	Simple root	$E_{k+1} \approx A\lvert E_k \rvert^{1.618}$
Newton-Raphson	Simple root	$E_{k+1} \approx A\lvert E_k \rvert^2$
Accelerated Newton-Raphson	Multiple root	$E_{k+1} \approx A\lvert E_k \rvert^2$