Numerical Calculus

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References

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Nonlinear Equations (Burden *et al.*, 2022)

Examples of nonlinear equations

$$x^2 + 7x - 4 = 0$$

$$\sin(x) + 2^{-x} = 0$$

$$\cos(x)\cosh(x) - 1 = 0$$

General form

$$f(x) = 0,$$

where f is a continuous function. In our cases $f(x) = x^2 + 7x - 4$, $f(x) = \sin(x) + 2^{-x}$, $f(x) = \cos(x)\cosh(x) - 1$.
Root-finding problem: determine a root/solution, α, of the equation (*zero* of the function f, $f(\alpha) = 0$)

Bisection or Binary search method (Gautschi, 2012)

Bisection method generates a sequence of nested intervals $[a_n, b_n]$, $n = 1, 2, \dots$; whereby each interval is guaranteed to contain at least one solution of the equation. As $n \to \infty$, the length of these intervals tends to 0, so that in the limit exactly one (isolated) root is *captured*. The method applies to any equation with f a continuous function, but has no built-in control of steering the iteration to any particular (real) solution if there is more than one.

Bisection Method (Burden *et al.*, 2022)

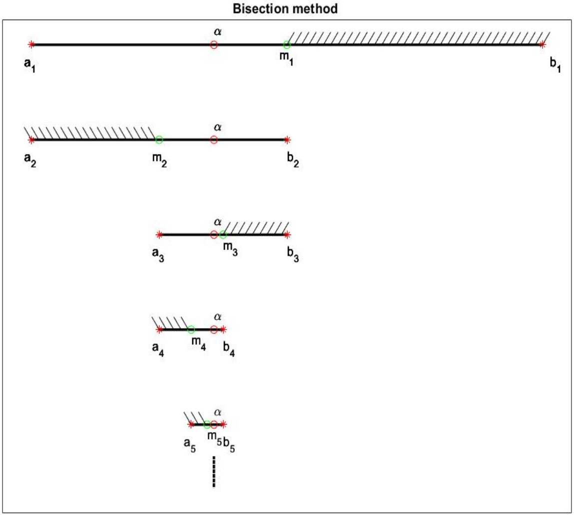
Let $\alpha \in (a, b)$ the solution of equation $f(x) = 0$ and let α_1 the midpoint of $[a, b]$

$$a_1 = a,\ b_1 = b,\ \alpha_1 = a_1 + \frac{b_1 - a_1}{2} = \frac{a_1 + b_1}{2}$$

- If $f(\alpha_1) = 0$, then $\alpha = \alpha_1$, and we are done.
- If $f(\alpha_1) \neq 0$ then $f(\alpha_1)$ has the same sign as either $f(a_1)$ or $f(b_1)$
  - If $f(\alpha_1)$ and $f(a_1)$ have the same sign $\Rightarrow \alpha \in (\alpha_1, b_1)$. Set $a_2 = \alpha_1$ and $b_2 = b_1$
  - If $f(\alpha_1)$ and $f(a_1)$ have opposite sign $\Rightarrow \alpha \in (a_1, \alpha_1)$. Set $a_2 = a_1$ and $b_2 = \alpha_1$

Then reapply the process to the interval $[a_2, b_2]$.

Bisection method



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Bisection method (Burden *et al.*, 2022)

Suppose $f \in C[a,b]$ and $f(a) \cdot f(b) < 0$. The bisection method generates a sequence $(\alpha_n)_n$ approximating a zero α of f with

$$|\alpha_n - \alpha| \leq \frac{1}{2}|b_n - a_n| = \frac{b-a}{2^n}, \quad \forall\, n \geq 1$$

Denoting by $e_n = |\alpha_n - \alpha|$ the *absolute error* at step n we have

$$e_n \leq \frac{b-a}{2^n} \Rightarrow \lim_{n\to\infty} e_n = 0$$

The bisection method is *globally convergent*. To get $e_n \leq \varepsilon$, where ε is a *fixed tolerance*, we must take

$$n \geq \frac{\ln \frac{b-a}{\varepsilon}}{\ln 2} \approx \frac{\ln \frac{b-a}{\varepsilon}}{0.6931}$$

Bisection method (Burden *et al.*, 2022)

Moreover, $|\alpha - \alpha_n| \leq (b-a)\frac{1}{2^n} \Rightarrow (\alpha_n)_n$ converges to α with the rate of convergence $O(\frac{1}{2^n})$, *i.e.*

$$\alpha_n = \alpha + O(\frac{1}{2^n}).$$

It is important to realize that previous inequality gives only a bound for approximation error and, in many cases, this bound is much larger. For example, $f(x) = x^3 + 4x^2 - 10$, $\alpha \in [1,2]$.

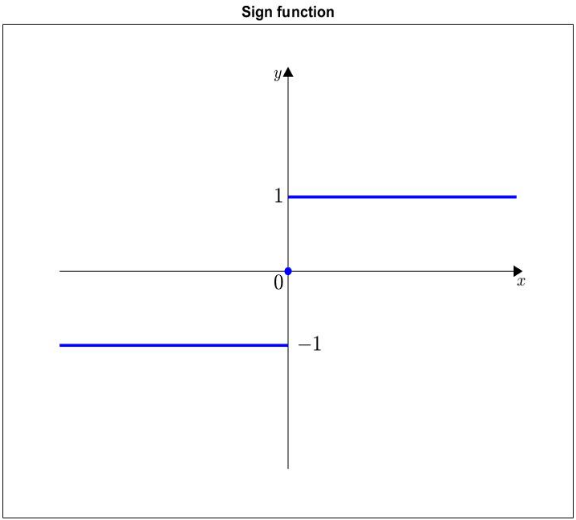
Bisection method (Burden *et al.*, 2022)

To determine which subinterval of $[a_n, b_n]$ contains a root of f, it is better to make use of the *signum function*, which is defined as

$$sign(x) = \begin{cases} -1, x < 0 \\ 0, x = 0 \\ 1, x > 0 \end{cases}$$

The test $sign(f(a_n))sign(f(b_n)) < 0$ instead of $f(a_n)f(b_n) < 0$ gives the same result but avoids the possibility of overflow or underflow in the multiplication of $f(a_n)$ and $f(b_n)$.

Sign function



Bisection method (Burden *et al.*, 2022)

When implementing the method on a computer, we need to consider the effects of round-off error. For example, the computation of the midpoint of the interval $[a_n, b_n]$ should be found from the equation

$$\alpha_n = a_n + \frac{b_n - a_n}{2} \text{ instead of } \alpha_n = \frac{a_n + b_n}{2}.$$

The first equation adds a small correction, $\frac{b_n - a_n}{2}$, to the known value a_n. When $b_n - a_n$, is near the maximum precision of the machine, this correction might be in error, but the error would not significantly affect the computed value of α_n. However, it is possible for $\frac{a_n + b_n}{2}$ to return a midpoint that is not even in the interval $[a_n, b_n]$.

Fixed-Point Iteration (Burden *et al.*, 2022)

The number α is a *fixed point* for a given function g if $g(\alpha) = \alpha$. Given a *root-finding problem* $f(\alpha) = 0$ we can define function g with a fixed point at α in a number of ways. For example,

$$g(x) = x - f(x).$$

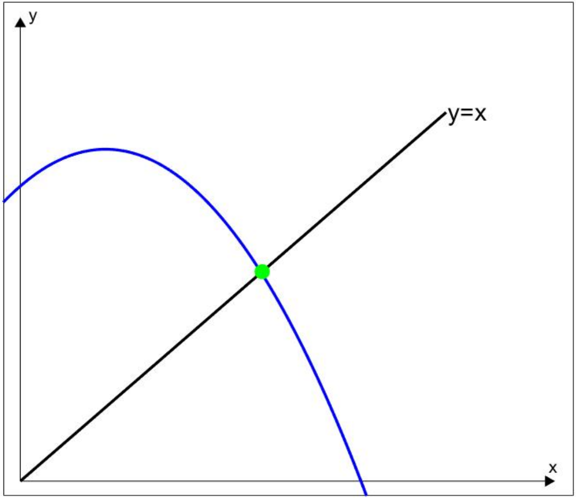
Conversely, if the function g has a fixed point at α, then the function defined by

$$f(x) = x - g(x)$$

has a zero at α.
A fixed point for g occurs precisely when the graph of $y = g(x)$ intersects the graph of $y = x$.

Fixed Point

FIXED POINT FOR A FUNCTION



Example (Burden *et al.*, 2022)

There are many ways to change the equation to the fixed-point form $x = g(x)$ using simple algebraic manipulation. For example, $\underbrace{x^3 + 4x^2 - 10}_{f(x):=} = 0$

$$x = g_1(x) = x - x^3 - 4x^2 + 10$$

$$x = g_2(x) = \left(\frac{10}{x} - 4x\right)^{\frac{1}{2}}$$

$$x = g_3(x) = \frac{1}{2}(10 - x^3)^{\frac{1}{2}}$$

$$x = g_4(x) = \left(\frac{10}{4+x}\right)^{\frac{1}{2}}$$

$$x = g_5(x) = x - \frac{x^3+4x^2-10}{3x^2+8x}$$

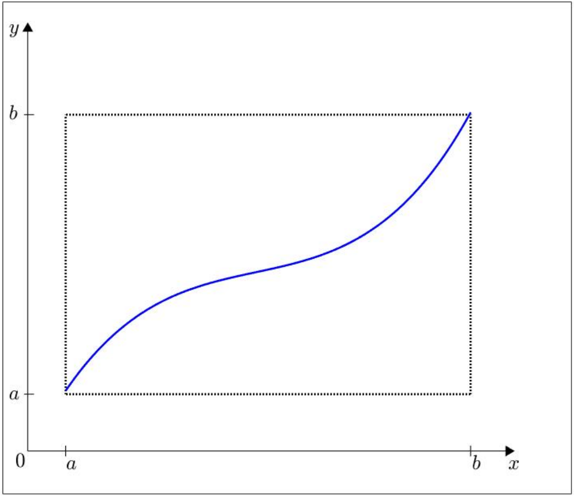
Fixed-Point Theorem (Burden *et al.*, 2022)

The existence and uniqueness of a fixed point.
If $g \in C[a, b]$ and $g(x) \in [a, b]\,(\mathrm{Im}(g) \subseteq [a, b])$ for all $x \in [a, b]$ then g has at least one fixed point in $[a, b]$.
If, in addition, $g'(x)$ exists on (a, b) and a constant $0 < k < 1$ exists with

$$|g'(x)| \leq k$$

for all $x \in (a, b)$ then there is exactly one fixed point in $[a, b]$.

$\mathrm{Im}(g) \subseteq [a, b]$



Fixed-Point Iteration (Burden *et al.*, 2022)

To approximate the fixed point of a function g, we choose an initial approximation $\alpha_0 \in (a, b)$ and generate the sequence $(\alpha_n)_n$ by letting

$$\alpha_n = g(\alpha_{n-1}), \; \forall \, n \geq 1.$$

If the sequence converges to α and g is continuous, then

$$\alpha = \lim_{n\to\infty} \alpha_n = \lim_{n\to\infty} g(\alpha_{n-1}) = g(\lim_{n\to\infty} \alpha_{n-1}) = g(\alpha)$$

and a solution to $x = g(x)$ is obtained. This technique is called *fixed-point* or *functional iteration.*

Convergence Result (Burden *et al.*, 2022)

Let $g \in C[a, b]$ and $g(x) \in [a, b]$ for all $x \in [a, b]$. Suppose, that in addition $g'(x)$ exists on (a, b) and a constant $0 < k < 1$ exists with

$$|g'(x)| \leq k$$

Then, for any number $\alpha_0 \in (a, b)$, the sequence defined by

$$\alpha_n = g(\alpha_{n-1}), \; \forall \, n \geq 1,$$

converges to the unique fixed point $\alpha \in [a, b]$.

Error estimates (Burden *et al.*, 2022)

The bounds for the error involved in using α_n to approximate α are given by

$$|\alpha_n - \alpha| \leq k^n \max\{\alpha_0 - a, b - \alpha_0\},$$

$$|\alpha_n - \alpha| \leq \frac{k^n}{1-k}|\alpha_1 - \alpha_0| \,(\textit{a priori} \text{ error estimate})$$

and

$$|\alpha_{n+1} - \alpha| \leq \frac{k}{1-k}|\alpha_{n+1} - \alpha_n| \,(\textit{a posteriori} \text{ error estimate})$$

Inequalities relate the rate at which $(\alpha_n)_n$ converges and bound k on the first derivative. The rate of convergence depends on the factor k^n. The smaller the value of k, the faster the convergence. The convergence may be very slow if k is close to 1.

Convergence Result (Burden *et al.*, 2022)

Let $g \in C^1[a, b]$ and α be in (a, b) with

$$g(\alpha) = \alpha \text{ and } |g'(\alpha)| > 1.$$

If $\exists\, \delta > 0$ s.t. $0 < |\alpha_0 - \alpha| < \delta$ then

$$|\alpha_0 - \alpha| < |\alpha_1 - \alpha|.$$

Thus, no matter how close the initial approximation α_0 is to α, the next iterate α_1 is farther away, so the fixed-point iteration does not converge if $\alpha_0 \neq \alpha$.

Order of convergence (Burden *et al.*, 2022)

Let $g \in C[a,b]$ and $g(x) \in [a,b], \forall\, x \in [a,b]$. Suppose, that in addition, $g' \in C(a,b)$ and $\exists\, k \in (0,1)$ s.t.

$$|g'(x)| \le k.$$

If $g'(\alpha) \ne 0$ then $\forall\, \alpha_0 \in [a,b]$, $\alpha_0 \ne \alpha$ the sequence

$$\alpha_n = g(\alpha_{n-1}),\ \forall\, n \ge 1$$

converges *only linearly* to the unique fixed point $\alpha \in [a,b]$. Moreover,

$$\lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|} = |g'(\alpha)|.$$

This result implies that higher-order convergence for fixed-point methods of the form $g(\alpha) = \alpha$ can occur only when $g'(\alpha) = 0$.

Order of convergence (Burden *et al.*, 2022)

Let α be a solution of the equation $x = g(x)$. Suppose that $g'(\alpha) = 0$ and $g'' \in C(a, b)$ with $|g''(x)| \leq M$ on an open interval I containing α. Then $\exists\, \delta > 0$ s.t. $\forall\, \alpha_0 \in [\alpha - \delta, \alpha + \delta]$ the sequence $\alpha_n = g(\alpha_{n-1})$ converges *at least quadratically* to α and

$$\lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^2} = \frac{|g''(\alpha)|}{2}.$$

Moreover, for sufficiently large values of n

$$|\alpha_{n+1} - \alpha| \leq \frac{M}{2} |\alpha_n - \alpha|^2.$$

Order of convergence (Burden *et al.*, 2022)

Higher-order one points method: Assume α is a fixed-point of g, $g(\alpha) = \alpha$, and g is p times continuously differentiable for all x near to α, for some $p \geq 2$. Furthermore, assume

$$g'(\alpha) = g''(\alpha) = \ldots = g^{(p-1)}(\alpha) = 0$$

If the initial guess α_0 is chosen sufficiently close to α, the iteration $\alpha_{n+1} = g(\alpha_n)$ will have order of convergence p, and

$$\lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^p} = \frac{|g^{(p)}(\alpha)|}{p!}.$$

Stopping Criteria. Control of the residual (Quarteroni *et al.*, 2000)

Suppose $(\alpha_n)_n$ is a sequence that converges to a zero α of f. Let

- ε a fixed tolerance on the approximate calculation
- $e_n = |\alpha - \alpha_n|$ the absolute error at step n.

Control of the residual: *the iterative process terminates at the first step n such that* $|f(\alpha_n)| \leq \varepsilon$

In the case of simple roots, the error is bound to the residual by the factor $\frac{1}{|f'(\alpha)|}$.

- If $|f'(\alpha)| \approx 1$ then $e_n \approx \varepsilon$ (the test provides a satisfactory indication of the error)
- If $|f'(\alpha)| \ll 1$ then the test is not reliable since e_n could be quite large with respect to ε
- If $|f'(\alpha)| \gg 1$ we get $e_n \ll \varepsilon$ an the test is too restrictive

Control of the increment (Quarteroni *et al.*, 2000)

Control of the increment: the iterative process terminates as soon as $|\alpha_{n+1} - \alpha_n| \leq \varepsilon$. Let $(\alpha_n)_n$ be generated by

$$\alpha_{n+1} = g(\alpha_n)$$

Using the mean value theorem we get

$$e_{n+1} = |\alpha - \alpha_{n+1}| = |g(\alpha) - g(\alpha_n)| = |g'(\xi_n)||\alpha - \alpha_n| = |g'(\xi_n)|e_n$$

where ξ_n lies between α_n and α. Then

$$\alpha_{n+1} - \alpha_n = (\alpha - \alpha_n) - (\alpha - \alpha_{n+1}) =$$

$$= (\alpha - \alpha_n) - (g(\alpha) - g(\alpha_n)) = (1 - g'(\xi_n))(\alpha - \alpha_n)$$

We replace $g'(\xi_n)$ with $g'(\alpha)$ and obtain

$$e_n \approx \frac{1}{|1 - g'(\alpha)|}|\alpha_{n+1} - \alpha_n|$$

Control of the increment (Quarteroni *et al.*, 2000)

If $g'(\alpha) \in (-1, 1)$ then $\frac{1}{1-g'(\alpha)} \in (\frac{1}{2}, \infty)$. We can conclude that the control of increment

- is unsatisfactory if $g'(\alpha)$ is close to 1
- provides an optimal balancing between increment and error in the case of methods of order 2 for which $g'(\alpha) = 0$ (as in the case of Newton method)
- is still satisfactory if $-1 < g'(\alpha) < 0$.

Accelerating Convergence. Aitken Δ^2 method (Burden *et al.*, 2022)

The technique called Aitken's Δ^2 method can be used to accelerate the convergence of a sequence that is linearly convergent.

Suppose $(\alpha_n)_n$ is a linearly convergent sequence with limit α. To motivate the construction of a sequence $(\hat{\alpha}_n)_n$ which converges more rapidly to α let us assume that the signs of $\alpha_n - \alpha$, $\alpha_{n+1} - \alpha$, and $\alpha_{n+2} - \alpha$ agree and that n is sufficiently large such that

$$\frac{\alpha_{n+1} - \alpha}{\alpha_n - \alpha} \approx \frac{\alpha_{n+2} - \alpha}{\alpha_{n+1} - \alpha}$$

Aitken Δ^2 method (Burden *et al.*, 2022)

$$\alpha \approx \frac{\alpha_{n+2}\alpha_n - \alpha_{n+1}^2}{\alpha_{n+2} - 2\alpha_{n+1} + \alpha_n} = \alpha_n - \frac{(\alpha_{n+1} - \alpha_n)^2}{\alpha_{n+2} - 2\alpha_{n+1} + \alpha_n}$$

Aitken Δ^2 method

$$\hat{\alpha}_n = \alpha_n - \frac{(\alpha_{n+1} - \alpha_n)^2}{\alpha_{n+2} - 2\alpha_{n+1} + \alpha_n}.$$

Forward difference

$$\begin{cases} \Delta\alpha_n = \alpha_{n+1} - \alpha_n, \; n \geq 0 \\ \Delta^k\alpha_n = \Delta(\Delta^{k-1}\alpha_n), \; k \geq 2. \end{cases}$$

Aitken Δ^2 method (Burden *et al.*, 2022)

In compact form

$$\hat{\alpha}_n = \alpha_n - \frac{(\Delta\alpha_n)^2}{\Delta^2\alpha_n}$$

Suppose that $(\alpha_n)_n$ converges linearly to the limit α

$$\lim_{n\to\infty} \frac{\alpha_{n+1} - \alpha}{\alpha_n - \alpha} < 1.$$

The Aitken's Δ^2 sequence $(\hat{\alpha}_n)_n$ converges to α faster than $(\alpha_n)_n$ in the sense that

$$\lim_{n\to\infty} \frac{\hat{\alpha}_n - \alpha}{\alpha_n - \alpha} = 0.$$

The Newton's method (Burden *et al.*, 2022)

There are many ways of introducing Newton's method. We can consider the technique based on Taylor polynomials. Suppose that $f \in C^2[a,b]$ and $\alpha_0 \in [a,b]$ be an approximation to α such that $f'(\alpha_0) \neq 0$ and $|\alpha - \alpha_0|$ is *small*.

$$\underbrace{f(\alpha)}_{=0} = f(\alpha_0) + (\alpha - \alpha_0) f'(\alpha_0) + \frac{(\alpha - \alpha_0)^2}{2!} f''(\xi(\alpha))$$

where $\xi(\alpha)$ lies between α and α_0.

$$0 = f(\alpha_0) + (\alpha - \alpha_0) f'(\alpha_0) + \frac{(\alpha - \alpha_0)^2}{2!} f''(\xi(\alpha))$$

The Newton's method (Burden *et al.*, 2022)

$$|\alpha - \alpha_0| \text{ is small } \Rightarrow (\alpha - \alpha_0)^2 \text{ is much smaller}$$

$$0 \approx f(\alpha_0) + (\alpha - \alpha_0) f'(\alpha_0) \Rightarrow \alpha \approx \alpha_0 - \frac{f(\alpha_0)}{f'(\alpha_0)} \equiv \alpha_1$$

This sets the stage for Newton's method, which starts with an initial approximation α_0 and generates the sequence $(\alpha_n)_n$

$$\alpha_n = \alpha_{n-1} - \frac{f(\alpha_{n-1})}{f'(\alpha_{n-1})}, \quad n \geq 1.$$

Newton's method is a functional iteration technique with

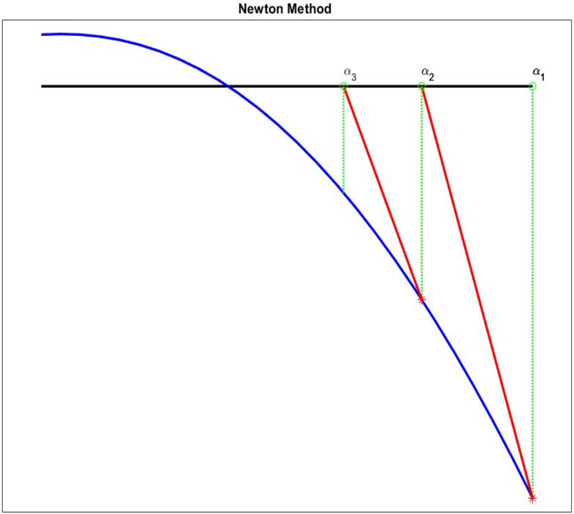
$$\alpha_n = g(\alpha_{n-1}), \text{ for witch } g(\alpha_{n-1}) = \alpha_{n-1} - \frac{f(\alpha_{n-1})}{f'(\alpha_{n-1})}$$

It is clear that Newton's method cannot be continued if $f'(\alpha_n) = 0$ for some n.

The Newton's method (Burden *et al.*, 2022)

The next figure illustrates how the approximations are obtained using successive tangents. Starting with the initial approximation α_1, the approximation α_2 is the x-intercept of the tangent line to the graph of f at $(\alpha_1, f(\alpha_1))$. The approximation α_2 is the x-intercept of the tangent line to the graph of f at $(\alpha_1, f(\alpha_1))$. The approximation α_3 is the x-intercept of the tangent line to the graph of f at $(\alpha_2, f(\alpha_2))$ and so on.

Newton method



The Newton's method (Burden *et al.*, 2022)

Let $f \in C^2[a, b]$. If $\alpha \in (a, b)$ s.t. $f(\alpha) = 0$ and $f'(\alpha) \neq 0$, then $\exists\, \delta > 0$ s.t. Newton's method generates a sequence $(\alpha_n)_n$ that converges to α, $\forall\, \alpha_0 \in [\alpha - \delta, \alpha + \delta]$.

This result is important for the theory of Newton's method, but it is rarely applied in practice because it does not tell us how to determine δ. In a practical application, an initial approximation is selected, and successive approximations are generated by Newton's method. Either these will generally converge quickly to the root, or it will be clear that convergence is unlikely.

The Newton's method (Dahlquist and Bjork, 2008)

Assume that α is a simple root of equation $f(x) = 0$, *i.e.*, $f'(\alpha) \neq 0$. If f' exists and is continuous in a neighborhood of α, then the convergence order of Newton's method is at least equal to two. Moreover,

$$\lim_{n \to \infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^2} = \underbrace{\frac{1}{2} \left| \frac{f''(\alpha)}{f'(\alpha)} \right|}_{\lambda =}$$

If $f''(\alpha) \neq 0$ then $\lambda > 0$ and the rate of convergence is quadratic.

The secant method (Burden *et al.*, 2022)

Newton's method is an extremely powerful technique, but it has a major weakness; the need to know the value of the derivative of f at each approximation. To circumvent the problem of the derivative evaluation in Newton's method, we introduce a slight variation. By definition,

$$f'(\alpha_{n-1}) = \lim_{x \to \alpha_{n-1}} \frac{f(x) - f(\alpha_{n-1})}{x - \alpha_{n-1}}$$

If α_{n-2} is close to α_{n-1} then

$$f'(\alpha_{n-1}) \approx \frac{f(\alpha_{n-2}) - f(\alpha_{n-1})}{\alpha_{n-2} - \alpha_{n-1}} = \frac{f(\alpha_{n-1}) - f(\alpha_{n-2})}{\alpha_{n-1} - \alpha_{n-2}}$$

Using this approximation for $f'(\alpha_{n-1})$ in Newton's formula gives

$$\alpha_n = \alpha_{n-1} - \frac{f(\alpha_{n-1})}{\frac{f(\alpha_{n-1}) - f(\alpha_{n-2})}{\alpha_{n-1} - \alpha_{n-2}}}.$$

The secant method (Burden *et al.*, 2022)

The following equivalent form is used in numerical computing

$$\alpha_n = \alpha_{n-1} - \frac{f(\alpha_{n-1})(\alpha_{n-1} - \alpha_{n-2})}{f(\alpha_{n-1}) - f(\alpha_{n-2})}.$$

Moreover, we have the compact form

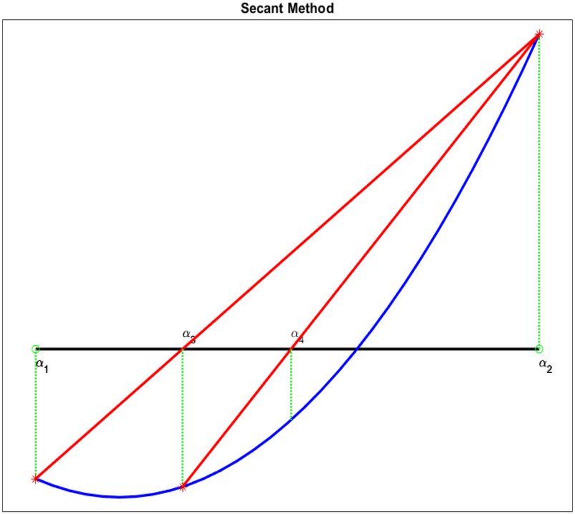
$$\alpha_n = \alpha_{n-1} - \frac{f(\alpha_{n-1})}{[\alpha_{n-2}, \alpha_{n-1}; f]}$$

where

$$[a, b; f] = \frac{f(b) - f(a)}{b - a}$$

represents the divided difference (see Lagrange Interpolation).

Secant method



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The secant method (Shampine *et al.*, 1997)

Note that although the secant method requires two initial approximations to the root, only one function evaluation per step is needed.

The secant rule with initial guesses α_0, α_1 converges to a simple zero α of f if α_0, α_1 lie in a sufficiently small closed interval containing α on which f', f'' exist and are continuous and $f'(x)$ does not vanish. Moreover,

$$\lim_{n \to \infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^p} \neq 0$$

where $p = \frac{1+\sqrt{5}}{2} \approx 1.618$.

The method of False Position (Burden *et al.*, 2022)

Each successive pair of approximations in the bisection method brackets a root α of the equation; that is, for each positive integer n, a root lies between a_n and b_n. Root bracketing is not guaranteed for either Newton's method or Secant method. The *False Position method* (also called *Regula Falsi*) generates approximations in the same manner as the Secant method, but includes a test to ensure that the root is always bracketed between successive iterations. First, choose initial approximations α_1 and α_2 with $f(\alpha_1) \cdot f(\alpha_2) < 0$.

The method of False Position (Burden *et al.*, 2022)

The approximation α_3 is chosen in the same manner as in the Secant method as the Ox-intercept of the line joining $(\alpha_1, f(\alpha_1))$ and $(\alpha_2, f(\alpha_2))$. To decide which secant line to use to compute α_4, consider $sign(f(\alpha_2))sign(f(\alpha_3))$.

- If $sign(f(\alpha_2))sign(f(\alpha_3)) < 0$, then α_2 and α_3 bracket a root. Choose α_4 as the Ox-intercept of the line joining $(\alpha_2, f(\alpha_2))$ and $(\alpha_3, f(\alpha_3))$.
- If not, choose α_4 as the Ox-intercept of the line joining $(\alpha_1, f(\alpha_1))$ and $(\alpha_3, f(\alpha_3))$ and then interchange the indices on α_1 and α_2.

In a similar manner, once α_4, is found, the sign of $f(\alpha_3)f(\alpha_4)$ determines whether we use α_3 and α_4, or α_2 and α_4 to compute α_5. In the latter case a relabeling of α_2 and α_3 is performed. The relabeling ensures that the root is bracketed between successive iterations.

Comparison of Newton's method and the secant method (Atkinson, 1989)

Newton's method and the secant method are closely related. If the approximation

$$f'(\alpha_n) \approx \frac{f(\alpha_n) - f(\alpha_{n-1})}{\alpha_n - \alpha_{n-1}}$$

is used in the Newton formula we obtain the secant formula. There are two major differences.

- Newton's method-requires-two function evaluations per iterate, that of $f(\alpha_n)$ and $f'(\alpha_n)$, whereas the secant method requires only one function evaluation per iterate, that of $f(\alpha_n)$ (provided the needed function value $f(\alpha_{n-1})$ is retained from the last iteration).
- Newton's method converges more rapidly (order $p = 2$) than secant method (order $p = \frac{1+\sqrt{5}}{2} \approx 1.618$).

Comparison of Newton's method and the secant method (Atkinson, 1989)

We now consider the expenditure of time necessary to reach a desired root α within a desired tolerance of ε. To simplify the analysis, we assume that the initial guesses are quite close to the desired root. Define

$$\alpha_{n+1} = \alpha_n - \frac{f(\alpha_n)}{f'(\alpha_n)},\ n \geq 0,\ c = \left|\frac{f''(\alpha)}{2f'(\alpha)}\right|$$

$$\bar{\alpha}_{n+1} = \bar{\alpha}_n - f(\bar{\alpha}_n)\frac{\bar{\alpha}_n - \bar{\alpha}_{n-1}}{f(\bar{\alpha}_n) - f(\bar{\alpha}_{n-1})},\ n \geq 1$$

and let $\alpha_0 = \bar{\alpha}_0$. We have

$$|\alpha - \alpha_{n+1}| \approx c|\alpha - \alpha_n|^2$$

$$|\alpha - \bar{\alpha}_{n+1}| \approx c^{r-1}|\alpha - \bar{\alpha}_n|^r,\ n \geq 0,\ r = \frac{1+\sqrt{5}}{2}$$

Comparison of Newton's method and the secant method (Atkinson, 1989)

Inductively for the error in the Newton iterates,

$$|\alpha - \alpha_n| \approx \frac{1}{c}(c|\alpha - \alpha_0|)^{2^n}$$

Similarly for the secant method iterates,

$$|\alpha - \bar{\alpha}_n| \approx \frac{1}{c}(c|\alpha - \alpha_0|)^{r^n}$$

To satisfy $|\alpha - \alpha_n| \leq \varepsilon$ for the Newton iterates, we must have

$$(c|\alpha - \alpha_0|)^{2^n} \leq c\varepsilon$$

$$\frac{K}{\ln 2} \leq n \text{ where } K = \ln\left(\frac{\ln(c\varepsilon)}{\ln(c|\alpha - \alpha_0|)}\right).$$

Comparison of Newton's method and the secant method (Atkinson, 1989)

Let m be the time to evaluate $f(x)$, and let $s \cdot m$ be the time to evaluate $f'(x)$. Then the minimum time to obtain the desired accuracy with Newton's method is

$$T_N = (m + ms)n = \frac{(1+s)mK}{\ln 2}.$$

For the secant method, a similar calculation shows that the minimum time necessary to obtain the desired accuracy is

$$T_S = mn = \frac{mK}{\ln r}.$$

To compare the times for the secant method and Newton's method, we have

$$\frac{T_S}{T_N} = \frac{\ln 2}{(1+s)\ln r}.$$

Comparison of Newton's method and the secant method (Atkinson, 1989)

The secant method is faster than the Newton method if the ratio is less than one,

$$\frac{T_S}{T_N} < 1 \Rightarrow s > \frac{\ln 2}{\ln r} - 1 = \frac{\ln 2}{\ln \frac{1+\sqrt{5}}{2}} - 1 \approx 0.44$$

If the time to evaluate $f'(x)$ is more than 44 percent of that necessary to evaluate $f(x)$, then the secant method is more efficient. In practice, many other factors will affect the relative costs of the two methods, so that the .44 factor should be used with caution. The preceding argument is useful in illustrating that the mathematical speed of convergence is not the complete picture.

Newton-Fourier Method (Atkinson, 1989)

Let $f \in C^2[a,b]$ s.t. $\alpha \in (a,b)$. Further we assume that

$$f(a) < 0,\ f(b) > 0,\ f'(x) > 0,\ f''(x) > 0,\ \forall\, x \in [a,b].$$

We have

f is strictly increasing on $[a,b]$

$\exists!\, \alpha \in [a,b]$ (unique solution)

$f(x) < 0,\ \forall\, x \in [a,\alpha)$ and $f(x) > 0,\ \forall\, x \in (\alpha, b]$

We consider $x_0 = b$, $z_0 = a$ and we define

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x)},\ \ z_{n+1} = z_n - \frac{f(z_n)}{f'(x_n)}.$$

Newton-Fourier Method (Atkinson, 1989)

We have

$(x_n)_n$ is strictly decreasing, $\lim_{n\to\infty} x_n = \alpha$

$(z_n)_n$ is strictly increasing, $\lim_{n\to\infty} z_n = \alpha$

Moreover,

$$\lim_{n\to\infty} \frac{x_{n+1} - z_{n+1}}{(x_n - z_n)^2} = \frac{f''(\alpha)}{2f'(\alpha)}$$

showing that the distance between x_n and z_n decreases quadratically with n.