Numerical Calculus

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References

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Gamma and Beta functions (Artin, 1964)

Gamma function: $\Gamma(a) = \int_0^\infty e^{-t} t^{a-1}\, dt,\ a > 0$

Beta function: $B(a,b) = \int_0^1 t^{a-1}(1-t)^{b-1}\, dt,\ a, b > 0$

1. $\Gamma(1) = 1$, $\Gamma(\frac{1}{2}) = \sqrt{\pi}$, $\Gamma(a+1) = a\Gamma(a)$
2. $\Gamma(n+1) = n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n,\ \forall\, n \in \mathbb{N}$
3. *Reflection formula* $\Gamma(a)\Gamma(1-a) = \frac{\pi}{\sin \pi a}$
4. $B(a,b) = B(b,a),\ B(a+1,b) = \frac{a}{a+b} B(a,b)$
5. $B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)},\ B(a, 1-a) = \frac{\pi}{\sin \pi a},\ B(\frac{1}{2}, \frac{1}{2}) = \pi$
6. $\displaystyle\int_0^\infty e^{-t^2}\, dt = \frac{\Gamma(\frac{1}{2})}{2} = \frac{\sqrt{\pi}}{2}$
7. *Wallis's integrals*

   $$W_n = \int_0^{\frac{\pi}{2}} \sin^n\theta\, d\theta = \int_0^{\frac{\pi}{2}} \cos^n\theta\, d\theta = \frac{1}{2} B(\frac{n+1}{2}, \frac{1}{2})$$

Algebraic Polynomials (Quarteroni *et al.*, 2000)

In general, the number of zeros of a function cannot be determined *a priori*. An exception is provided by polynomials for which the number of zeros (real or complex) coincides with the degree of the polynomial.
The Abel theorem guarantees that there does not exist an explicit form to compute all zeros of a generic polynomial of degree $n \geqslant 5$. This fact further motivates the use of numerical methods for computing the roots.

$\mathbb{R}[X]$-the set of all polynomial with real coefficients

$\mathbb{C}[X]$-the set of all polynomial with real coefficients

$\Pi_n \subset \mathbb{R}[X]$-the set of polynomials having degree n or less

Polynomial of degree n (Quarteroni *et al.*, 2000)

Standard form

$$P_n(x) = \sum_{k=0}^{n} a_{n-k} x^{n-k} = a_n x^n + \ldots + a_1 x + a_0$$

Using roots $x_i \quad (P_n(x_i) = 0)$

$$P_n(x) = a_n (x - x_1)^{m_1} \ldots (x - x_k)^{m_k}, \sum_{i=1}^{k} m_i = n$$

Nested multiplications

$$P_n(x) = ((\ldots(a_n x + a_{n-1})x + a_{n-2})x + \ldots + a_2)x + a_1)x + a_0$$

Shifted power basis

$$P_n(x) = \sum_{k=0}^{n} b_{n-k} (x - c)^{n-k} = b_n (x - c)^n + \ldots + b_1 (x - c) + b_0$$

Fundamental Theorem of Algebra (Burden *et al.*, 2022)

Let the polynomial $P_n \in \Pi_n$ of degree n

$$P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a_0$$

If P_n is a polynomial of degree $n \geqslant 1$ with real or complex coefficients then P_n has at least one (possibly complex) root.

If P_n is a polynomial of degree $n \geqslant 1$ with real or complex coefficients, then there exist unique constants $x_1, x_2, \ldots, x_k \in \mathbb{C}$ and $m_1, m_2, \ldots, m_k \in \mathbb{N}$, s.t.

$$\sum_{i=1}^{k} m_i = n$$

and

$$P_n(x) = a_n (x - x_1)^{m_1} (x - x_2)^{m_2} \ldots (x - x_k)^{m_k}$$

(A polynomial of degree n has exactly n zeros.)

Zeros of Polynomials (Burden *et al.*, 2022)

Let P, $Q \in \Pi_n$ (polynomials of degree at most n). If $x_1, \ldots, x_k$ with $k > n$, are distinct numbers with

$$P(x_i) = Q(x_i), \forall\, i = 1, \ldots, k$$

then

$$P(x) = Q(x), \forall\, x.$$

This result implies that to show that two polynomials of degree less than or equal to n are the same, we need only to show that they agree at $n+1$ values.
Moreover, should $\alpha = x + yi$ with $y \neq 0$ be a zero of a polynomial with degree $n \geqslant 2$, if a_k are real coefficients, then its complex conjugate $\bar{\alpha} = x - yi$ is also a zero.

Polynomial Division. Horner's Algorithm (Quarteroni *et al.*, 2000; Burden *et al.*, 2022)

Given two polynomials $h \in \Pi_n$ and $g \in \Pi_m$ with $m \leqslant n$ there exist two unique polynomials $\delta \in \Pi_{n-m}$ and $\rho \in \Pi_{m-1}$ s.t.

$$h = g \cdot \delta + \rho,$$

$$0 \leqslant \deg(\rho) \leqslant \deg(g) - 1$$

Horner's method incorporates a nesting technique for efficiently evaluating a polynomial (and its derivative) at a given point α.

Horner's Algorithm (Quarteroni *et al.*, 2000; Burden *et al.*, 2022)

The *nested multiplications*

$$P_n(x) = ((\ldots(a_n x + a_{n-1})x + a_{n-2})x + \ldots + a_2)x + a_1)x + a_0$$

is the basic ingredient of Horner's method. This method efficiently evaluates the polynomial P_n at a point α through the following *synthetic division* algorithm

$$\begin{cases} b_n = a_n \\ b_k = a_k + b_{k+1}\alpha, \; \forall\, k = n-1, n-2, \ldots, 0 \end{cases}$$

All the coefficients b_k, $k \leqslant n-1$, depend on α and $b_0 = P_n(\alpha)$.

Horner's Algorithm (Quarteroni *et al.*, 2000)

The polynomial

$$Q_{n-1}(x,\alpha) = b_n x^{n-1} + \ldots + b_2 x + b_1 = \sum_{k=1}^{n} b_k x^{k-1}$$

of degree $n-1$ in x depends on the α parameter (through the coefficients b_k) and is called *associated polynomial* of P_n.
Dividing P_n by $x-\alpha$ it follows that

$$P_n(x) = (x-\alpha) Q_{n-1}(x;\alpha) + b_0, \text{ where } \alpha_0 = P_n(\alpha)$$

Horner's Algorithm. Deflation procedure (Quarteroni *et al.*, 2000; Burden *et al.*, 2022)

If α is a root of P_n then $b_0 = P_n(\alpha) = 0$ and

$$P_n(x) = (x - \alpha)Q_{n-1}(x; \alpha).$$

The algebraic equation $Q_{n-1}(x; \alpha) = 0$ provides the $n - 1$ remaining roots of P_n.
Deflation Procedure (for finding the roots of P_n):
For $m = n, n - 1, \ldots, 1$

1. Find a root α_m of P_m using a suitable approximation method;
2. Evaluate $Q_{m-1}(x; \alpha_m)$;
3. Set $P_{m-1} = Q_{m-1}$.

Rolle's Theorem. Generalized Rolle's Theorem (Burden *et al.*,2022)

Suppose $f \in C[a,b]$ and f is differentiable on (a,b). If $f(a) = f(b)$ then a number $c \in (a,b)$ exists with $f'(c) = 0$.

Suppose that $f \in C[a,b]$ is n times differentiable on (a,b). If $f(x) = 0$ at $(n+1)$ distinct numbers $a \leqslant x_0 < x_1 < \ldots < x_n \leqslant b$ then a number $c \in (a,b)$ exists with $f^{(n)}(c) = 0$.

If the function f is differentiable at x_0, then f is continuous at x_0.

Mean Value Theorem. Extreme Value Theorem (Burden *et al.*, 2022)

If $f \in C[a,b]$ and f is differentiable on (a,b), then a number c in (a,b) exists with

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$

If $f \in C[a,b]$, then $c_1, c_2 \in [a,b]$ exist with $f(c_1) \leqslant f(x) \leqslant f(c_2)$, for all $x \in [a,b]$. In addition, if f is differentiable in (a,b), then the numbers c_1 and c_2 occur either at the endpoints of $[a,b]$ or where f' is zero.

Intermediate value theorem (Burden *et al.*, 2022)

If $f \in C[a, b]$ and β is any number between $f(a)$ and $f(b)$ then there exists a number $\alpha \in (a, b)$ such that $f(\alpha) = \beta$.

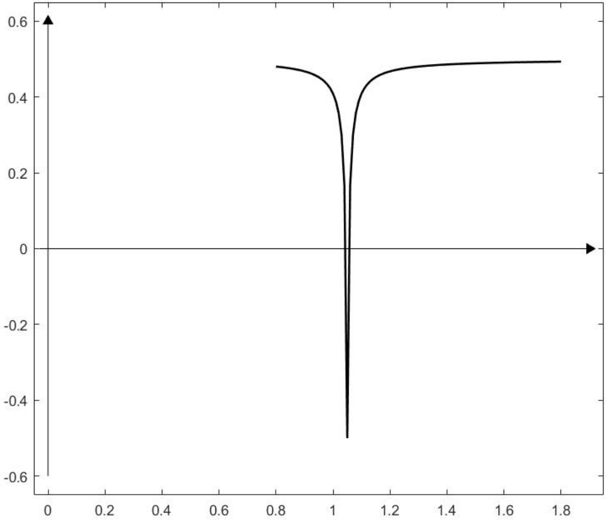
Particular case $\beta = 0$: $f \in C[a, b]$ with $f(a)$ and $f(b)$ of opposite sign $\Rightarrow \exists\, \alpha \in (a, b)$ with $f(\alpha) = 0$

However, finding such sub-intervals may not always be easy (Süli and Mayers, 2003)

$$f(x) = \frac{1}{2} - \frac{1}{1 + m|x - 1.05|}, \quad |m| \gg 0$$

$$x_1 = 1.05 - \frac{1}{m}, \quad x_2 = 1.05 + \frac{1}{m}$$

Graph of the function $f(x) = \frac{1}{2} - \frac{1}{1+200|x-1.05|}$, $x \in [0.8, 1.8]$



Weighted Mean Value Theorem for Integrals (Burden *et al.*, 2022)

Suppose $f \in C[a, b]$, the Riemann integral of g exists on $[a, b]$, and $g(x)$ does not change sign on $[a, b]$. Then there exists a number c in (a, b) with

$$\int_a^b f(x)g(x)\,dx = f(c)\int_a^b g(x)\,dx.$$

When $g \equiv 1$ is the usual Mean Value Theorem for Integrals. It gives the average value of the function over the interval $[a, b]$ as

$$f(c) = \frac{1}{b-a}\int_a^b f(x)\,dx.$$

Taylor's Theorem (Burden *et al.*, 2022)

Suppose $f \in C^n[a, b]$, $f^{(n+1)}$ exists on $[a, b]$ and $x_0 \in [a, b]$. For every $x \in [a, b]$ there exists $\xi(x)$ between x_0 and x with

$$f(x) = P_n(x) + R_n(x)$$

where

$$P_n(x) = f(x_0) + \frac{f'(x_0)}{1!}(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \\ + \ldots + \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k$$

and

$$R_n(x) = \frac{f^{n+1}(\xi(x))}{(n+1)!}(x - x_0)^{n+1}$$

Taylor Polynomials (Burden *et al.*, 2022)

P_n is called the *nth Taylor polynomial* for f about x_0, and R_n is called the *remainder term (or truncation error)* associated with P_n.

The Taylor polynomials agree as closely as possible with a given function at a specific point, but they concentrate their accuracy near that point. A good approximating polynomial needs to provide relative accuracy over an entire interval, and Taylor polynomials generally do not do this.

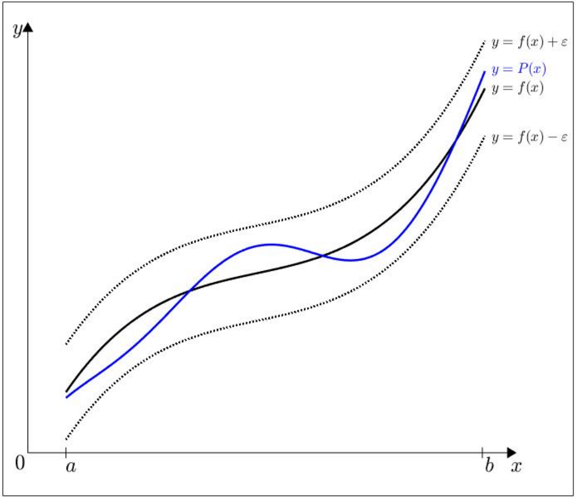
Weierstrass Approximation Theorem (Burden *et al.*, 2022)

Suppose f is a real function defined and continuous on $[a, b]$. For each $\varepsilon > 0$, there exists a polynomial P, with the property that

$$|f(x) - P(x)| \leqslant \varepsilon, \quad \forall\, x \in [a, b].$$

An important reason for considering the class of polynomials in the approximation of functions is that the derivative and indefinite integral of a polynomial are easy to determine and are also polynomials.

Weierstrass Approximation Theorem



Contraction (Süli and Mayers, 2003)

Suppose that $g : [a, b] \to [a, b]$ is a function, defined and continuous on a bounded closed interval $[a, b]$ of the real line. Then, g is said to be a *contraction* on $[a, b]$ if there exists a constant L such that $0 < L < 1$ and the *Lipschitz condition* holds

$$|g(x) - g(y)| \leqslant L|x - y|, \quad \forall\, x, y \in [a, b].$$

Condition can be rewritten in the following equivalent form

$$\left|\frac{g(x) - g(y)}{x - y}\right| \leqslant L, \quad \forall\, x, y \in [a, b],\ x \neq y$$

Contraction (Süli and Mayers, 2003)

Assuming that g is a differentiable function on the open interval (a, b) the Mean Value Theorem tells us that

$$\frac{g(x) - g(y)}{x - y} = g'(\eta), \quad \eta \in (x, y)$$

We shall therefore adopt the following assumption that is somewhat stronger but is easier to verify in practice

g is differentiable on (a, b)

$\exists\, 0 < L < 1$ s.t. $|g'(x)| \leqslant L \quad \forall\, x \in (a, b)$

Rates of Convergence (Burden *et al.*,2022)

Suppose $(\beta_n)_n$ is a sequence known to converge to zero and $(\alpha_n)_n$ converges to $\alpha \in \mathbb{R}$. If a positive constant K exists with

$$|\alpha_n - \alpha| \leqslant K|\beta_n|$$

for large n, then we say that $(\alpha_n)_n$ converges to α with rate, or order, of convergence of $O(\beta_n)$. It is indicated by writing $\alpha_n = \alpha + O(\beta_n)$. In nearly every situation we use

$$\beta_n = \frac{1}{n^p}$$

for some $p > 0$ and we write

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

Rates of Convergence (Burden *et al.*,2022)

Suppose that $\lim_{h\to 0} G(h) = 0$ and $\lim_{h\to 0} F(h) = L$. If a positive constant K exists with

$$|F(h) - L| \leqslant |G(h)|$$

for sufficiently small h, then we write

$$F(h) = L + O(G(h)).$$

The functions we use for comparison generally have the form $G(h) = h^p$, where $p > 0$. We are interested in the largest value of p for which

$$F(h) = L + O(h^p).$$

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

We consider a sequence $(\alpha_n)_n$ and assume that $\alpha_n \to \alpha$ and $\alpha_n \neq \alpha$, $\forall n \in \mathbb{N}$. If constants $0 \leqslant \lambda$ and $p \geqslant 1$ exist with

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

then $(\alpha_n)_n$ *converges to* α *of order p with asymptotic error constant* λ.

In general, a sequence with a high order of convergence converges more rapidly than a sequence with a lower order. The asymptotic constant affects the speed of convergence, but not to the extent of the order.

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

Special cases

$p = 1$, $\lambda < 1$: the sequence is *linearly convergent*

$p = 2$: the sequence is *quadratically convergent*

A sequence $(\alpha_n)_n$ is said to be *superlinearly convergent* to α if

$$\lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|} = 0\,(\lambda = 0, p = 1)$$

A sequence $(\alpha_n)_n$ is said to be *sublinear convergent* to α if

$$\lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|} = 1\,(\lambda = 1, p = 1)$$

If $\alpha_n \to \alpha$ of order p for $p > 1$ then $(\alpha_n)_n$ is superlinearly convergent to α. The sequence $\alpha_n = \frac{1}{n^n}$ converges superlinearly to 0 but does not convergence to 0 of order p for any $p > 1$.

(Dahlquist and Björk, 2008)

Examples

- sublinear: $x_n = \frac{1}{n} \to 0$
- linear: $x_n = \frac{1}{2^n} \to 0$
- superlinear: $x_n = \frac{1}{n^n} \to 0$
- quadratic: $x_0 > 0, c > 0,\ x_{n+1} = \frac{1}{2}(x_n + \frac{c}{x_n}),\ x_n \to \sqrt{c}$
- cubic: $x_0 > 0, c > 0,\ x_{n+1} = \frac{x_n(x_n^2+3c)}{3x_n^2+c},\ x_n \to \sqrt{c}$