Supplementary Material

Derivation of Taylor Series for erf

Recall the error function is defined as

$$\mathrm{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x .e^{-t^2} dt \tag{1}$$

The Taylor series expanded about $t = 0$ for e^{-t^2} is given as

$$e^{-t^2} = 1 - t^2 + \frac{t^4}{2} - \frac{t^6}{6} + \cdots = \sum_{k=0}^{\infty} (-1)^k \frac{t^{2k}}{k!} \tag{2}$$

The power series is uniformly convergent on $\mathbb{R}$, therefore it is also uniformly convergent on $[0, x]$. Using this fact to interchange the summation and integral we find

$$\begin{aligned}
\int_0^x e^{-t^2} dt &= \int_0^x \left(\sum_{k=0}^{\infty} (-1)^k \frac{t^{2k}}{k!} \right) dt \\
&= \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \left(\int_0^x t^{2k} dt \right) \\
&= \sum_{k=0}^{\infty} \left[\frac{(-1)^k t^{2k+1}}{k!(2k+1)} \right]_0^x \\
&= \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k+1}}{k!(2k+1)}.
\end{aligned}$$

Thus, we arrive at the Taylor series for erf

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k+1}}{k!(2k+1)}. \tag{3}$$

If we truncate the power series after the x^{2N+1} term, i.e. the upper limit of the summation is N, the first neglected term is

$$\frac{2}{\sqrt{\pi}} \frac{(-1)^{N+1} x^{2N+3}}{(N+1)!(2N+3)}. \tag{4}$$

For fixed $x > 0$, define

$$a_k(x) = \frac{x^{2k+1}}{k!(2k+1)} > 0. \tag{5}$$

Consider the ratio

$$\frac{a_{k+1}(x)}{a_k(x)} = \frac{(2k+1)}{(k+1)(2k+3)} x^2. \tag{6}$$

Therefore if the condition

$$\frac{(2N+1)}{(N+1)(2N+3)} x^2 < 1, \tag{7}$$

the terms in the Taylor series for $k = N+1,\ N+2, ...$ are alternating and decreasing so the absolute error is bounded by the first neglected term, i.e.

$$|\varepsilon_N(x)| \leqslant \frac{2}{\sqrt{\pi}} \frac{x^{2N+3}}{(N+1)!(2N+3)}. \tag{8}$$

This is automatically satisfied for small x, but N must be sufficiently large for larger x. In practice, the rounding error significantly outweighs the truncation error for larger x, so we can safely take this to be an upper bound for the truncation error in the regions that this series is applied, i.e $x \lesssim 2$.

Padé Approximation

An alternative to the Taylor series is a rational approximation in which we approximate the function using the ratio of two polynomials. The $[m/n]$ Padé approximation to a function f is a rational function

$$r(x) = \frac{p_0 + p_1 x + \cdots + p_m x^m}{q_0 + q_1 x + \cdots + q_n x^n}[1]. \tag{9}$$

We set $q_0 = 1$, and the remaining $m + n + 1$ coefficients are chosen such that

$$f^{(k)}(0) = r^{(k)}(0) \quad \text{for } k = 0, 1, ..., m+n[1]. \tag{10}$$

Equation (9) and (10) are equivalent to the expression

$$(a_0 + a_1 x + \cdots)(1 + q_1 x + \cdots q_n x^2) - (p_0 + p_1 x + \cdots p_m x^m) \tag{11}$$

having no terms of degree $\leqslant N := m + n$, where $\{a_k\}$ are the Taylor coefficients of f.

For convenience, we set $p_{m+1} = p_{m+2} = \cdots = p_N = 0$ and $q_{n+1} = q_{n+2} = \cdots = q_N = 0$.

The condition stated in Equation (11) can be written as the linear system

$$\sum_{i=0}^{k} a_i q_{k-i} = p_k, \qquad k = 0,\ 1,\ ...,\ N. \tag{12}$$

For $k = m+1,\ m+2,\ ..., N$, $p_k = 0$, which gives

$$\sum_{j=1}^{n} a_{k-j} q_j = -a_k. \tag{13}$$

This is a system of n linear equations in n unknowns.

After using Equation (13) to find $q_1,\ ...,\ q_n$, we can then use Equation (12) for $k = 0,\ 1,\ ...,\ m$ to calculate $p_0,\ ...,\ p_m$ directly.

When tested on the error function against the Taylor series, Padé approximation perform equally well on small values of x and better for larger x. However, the method fails to achieve the desired accuracy of $10\varepsilon_{\text{mach}}$ beyond $x \approx 3$. Therefore we do not explore this approximation further.

Bibliography

[1] Burden, R. L., Faires J. D., and Burden, A. M. (2015). Numerical Analysis. (10th ed). Cengage Learning.