Question
The error function $\text{erf}(x)$ is defined by

$$\text{erf}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\, dt$$

and is used widely, for example in probability (it's effectively the cumulative normal distribution) and in boundary layer flow in fluid dynamics. In this question we prove the Poincaré asymptotic expansion as $x \to +\infty$.

(i) By writing $e^{-t^2} = te^{-t^2} \times \frac{1}{t}$, use integration by parts to show that

$$\sqrt{\pi}(1 - \text{erf}(x)) = \frac{e^{-x^2}}{x} - \int_x^\infty \frac{e^{-t^2}}{t^2}\, dt$$

(ii) Given that $\sqrt{\pi} \times \left(\frac{1}{2}\right) \times \left(\frac{3}{2}\right) \times \left(\frac{5}{2}\right) \times \cdots \times \left(\frac{2n-1}{2}\right) = \Gamma\left(n + \frac{1}{2}\right)$ iterate this approach to show that

$$\begin{aligned} \sqrt{\pi}(1 - \text{erf}(x)) &= \frac{e^{-x^2}}{\sqrt{\pi}} \left[\sum_{r=0}^{n} \Gamma\left(r + \frac{1}{2}\right) \frac{(-1)^r}{x^{2r+1}}\right] + R_n(x) \\ R_n(x) &= -\Gamma\left(n + \frac{1}{2}\right)(2n+1)\frac{(-1)^n}{\sqrt{\pi}} \int_x^\infty \frac{e^{-t^2}}{t^{2n+2}}\, dt \end{aligned}$$

(iii) By comparing the integrand of the remainder integral with te^{-t^2} show that

$$|R_n(x)| \leq \frac{(2n+1)\Gamma\left(n + \frac{1}{2}\right)}{x^{2n+1}\sqrt{\pi}} \int_x^\infty te^{-t^2}\, dt$$

(iv) Hence show that

$$\pi e^{x^2}(1 - \text{erf}(x)) \sim \sum_{r=0}^{\infty} \Gamma\left(r + \frac{1}{2}\right) \frac{(-1)^r}{x^{2r+1}},\ x \to +\infty$$

and so deduce that

$$\text{erf}(x) \sim 1 - \frac{e^{-x^2}}{\pi} \sum_{r=0}^{\infty} \Gamma\left(r + \frac{1}{2}\right) \frac{(-1)^r}{x^{2r+1}},\ x \to +\infty$$

(v) For different truncations N use the above approximation to estimate the value of erf for $x = 2$, comparing it with the (numerically obtained) exact result of $\text{erf}(2) = 0.9953222650189\cdots$ Which truncation gives the best agreement? Can you explain what happens for higher truncations?

Answer

(i) $\text{erf}(x) = 1 - \dfrac{2}{\sqrt{\pi}} \displaystyle\int_x^\infty e^{-t^2}\, dt$

$$\begin{aligned}
\Rightarrow \sqrt{\pi}(1 - \text{erf}(x)) &= 2\int_x^\infty e^{-t^2}\, dt \\
&= 2\int_x^\infty \underbrace{\frac{1}{t}}_{\text{diff}} \underbrace{te^{-t^2}}_{\text{int}}\, dt \\
&= 2\left\{\left[\frac{-e^{-t^2}}{2t}\right]_x^\infty - \frac{1}{2}\int_x^\infty \frac{e^{-t^2}}{t^2}\, dt\right\} \\
&= \frac{e^{-x^2}}{x} - \int_x^\infty \frac{e^{-t^2}}{t^2}\, dt
\end{aligned}$$

(ii) $\sqrt{\pi}(1 - \text{erf}(x)) = \dfrac{e^{-x^2}}{x} - \displaystyle\int_x^\infty \frac{1}{t^3} te^{-t^2}\, dt$

$$= \frac{e^{-x^2}}{x} + \frac{1}{2}\left[\frac{1}{t^3}e^{-t^2}\right]_x^\infty + \frac{3}{2}\int_x^\infty \frac{1}{t^5}te^{-t^2}\, dt$$

$$= \frac{e^{-x^2}}{x} - \frac{e^{-x^2}}{2x^3} - \frac{3}{2}\cdot\frac{1}{2}\left[\frac{1}{t^5}e^{-t^2}\right]_x^\infty - \frac{3}{2}\cdot\frac{5}{2}\int_x^\infty \frac{1}{t^7}te^{-t^2}\, dt$$

$$= e^{-x^2}\left[\frac{1}{x} - \frac{1}{2x^3} + \frac{-1}{2}\cdot\frac{-3}{2}\frac{1}{x^5}\right] + \left(\frac{-1}{2}\right)\left(\frac{-3}{2}\right)(-5)\int_x^\infty \frac{1}{t^7}te^{-t^2}\, dt + \cdots$$

$$= e^{-x^2}\left[\frac{1}{x} - \frac{1}{2x^3} + \left(\frac{-1}{2}\right)\left(\frac{-3}{2}\right)\left(\frac{1}{x^5}\right) + \cdots + \left(\frac{-1}{2}\right)\left(\frac{-3}{2}\right) + \cdots \right.$$

$$\left. + \left(\frac{-[2n+1]}{2}\right)\frac{1}{x^{2n+1}}\right]$$

$$+ \left(\frac{-1}{2}\right)\left(\frac{-3}{2}\right) + \cdots + \left(\frac{-[2n-1]}{2}\right)(-[2n+1]) \times \int_x^\infty \frac{1}{t^{2n+1}}te^{-t^2}\, dt$$

$$= \frac{e^{-x^2}}{\sqrt{\pi}} \sum_{r=0}^{n} \frac{(-1)^r \Gamma(r + \frac{1}{2})}{x^{2r+1}} \; (\star) + R_n(x)$$

(using result given on Γ functions.)

$$R_n(x) = -\frac{\Gamma(n+\frac{1}{2})(2n+1)}{\sqrt{\pi}}(-1)^n \int_x^\infty \frac{e^{-t^2}}{t^{2n+2}}\,dt$$

(iii) Consider

$$\begin{aligned} |R_n(x)| &= \frac{\Gamma(n+\frac{1}{2})(2n+1)}{\sqrt{\pi}} \left| \int_x^\infty \frac{e^{-t^2}}{t^{2n+2}}\,dt \right| \\ &\quad \left(\Gamma\left(n+\tfrac{1}{2}\right) > 0 \text{ for } n > 0\right) \\ &\leq \frac{\Gamma(n+\frac{1}{2})}{\sqrt{\pi}}(2m+1) \int_x^\infty \left| \frac{e^{-t^2}}{t^{2n+2}} \right| dt \end{aligned}$$

For $x > 0$ $\left| \frac{e^{-t^2}}{t^{2n+2}} \right| = \frac{e^{-t^2}}{t^{2n+2}}$

Now $\frac{e^{-t^2}}{t^{2n+2}} = \frac{1}{t^{2n+3}} t e^{-t^2} \leq \frac{t e^{-t^2}}{x^{2n+3}}$ for $\underline{t > x\ (> 0)}$

$$\begin{aligned} \text{Therefore } |R_n(x)| &\leq \frac{\Gamma(n+\frac{1}{2})(2n+1)}{\sqrt{\pi}} \int_x^\infty \frac{t e^{-t^2}}{x^{2n+3}}\,dt \\ \Rightarrow |R_n(x)| &\leq \frac{\Gamma(n+\frac{1}{2})(2n+1)}{x^{2n+3}\sqrt{\pi}} \int_x^\infty t e^{-t^2}\,dt \end{aligned}$$

(iv) From this result

$$|R_n(x)| \leq \frac{\Gamma(n+\frac{1}{2})(2n+1)}{x^{2n+3}\sqrt{\pi}} \frac{e^{-x^2}}{2}$$

This is then

$$R_n(x) = O\left(\frac{e^{-x^2}}{x^{2n+3}}\right)$$

which is of the order of the first neglected term in the series ($\star$) above, as $x \to +\infty$.

Hence the series ($\star$) is Poincaré asymptotic as $x \to +\infty$.

Therefore $\sqrt{\pi}(1 - \text{erf}(x)) \sim \frac{e^{-x^2}}{\sqrt{pi}} \sum_{r=0}^{\infty} \frac{(-1)^r \Gamma(r+\frac{1}{2})}{x^{2r+1}},\ x \to +\infty$

or $\text{erf}(x) \sim 1 - \frac{e^{-x^2}}{\pi} \sum_{r=0} \infty \frac{(-1)^r \Gamma(r+\frac{1}{2})}{x}^{2r+1},\ x \to +\infty$

(v) Let truncation $= n$

$$|\text{Relative \% error}| = \left|1 - \frac{\text{approx}}{\text{exact}}\right| \times 100$$

n	approx	|rel. % err|	
0	$0.99_{\uparrow}4833257$	0.0491	Error decreases
1	$0.995_{\uparrow}479079$	0.158	
2	$0.995_{\uparrow}2369057$	0.0086	
3	$0.9953_{\uparrow}882752$	0.0066	

(Best approximation for $x = 2$ is when $n = 3$.)

4	0.9952558269	0.0067	Error increases
5	0.9954048313	0.0083	
6	0.9951999503	0.0123	
7	0.9955328819	0.0212	
8	0.9949086351	0.0416	
9	0.9962351596	0.0917	
10	0.9930846639	0.225	
⋮			
20	0.9953222950189	120,000% error!	
EXACT	0.9953222650189	0	

THE SERIES IS DIVERGENT! (for all x) (via e.g., ratio test), but excellent agreement initially. This can be explained by looking at the size of the terms $\dfrac{\Gamma\left(r+\frac{1}{2}\right)}{2^{2r}}$ for $r = 0 \cdots$.

r	$\left\lvert\dfrac{\Gamma\left(r+\frac{1}{2}\right)}{2^{2r}}\right\rvert$	
0	1.772	Terms decrease in size
1	0.222	
2	0.083	
3	0.052	
4	0.045	
5	0.051	Terms increase in size
5	0.070	
7	0.114	
8	0.214	

As $|R_n| = 0$ (1st neglected term) we see $|R_n|$ decreases to a minimum at $n \approx 4$ before increasing indefinitely.