Notes of a Numerical Analyst

Hermite polynomial surprises

NICK TREFETHEN FRS

Among the oldest tools in the box are Hermite polynomials, which are used for working with functions of a real variable that decay as $|x| \to \infty$. Hermite polynomial expansions and numerical methods are derived from conditions of optimality. Yet they are far — very far! — from optimal.

We can illustrate the issue by looking at a problem of quadrature. Suppose a function f is given and we want to calculate the integral

$$I = \int_{-\infty}^{\infty} f(x) e^{-x^2} dx. \qquad (1)$$

A quadrature formula is an approximation

$$I_n = \sum_{k=1}^{n} w_k f(x_k) \qquad (2)$$

for some nodes $x_1, \ldots, x_n$ and weights $w_1, \ldots, w_n$. Suppose we ask, what $\{x_k\}$ and $\{w_k\}$ are optimal in the sense that (2) gives exactly the correct answer, $I = I_n$, whenever f is a polynomial of the highest possible degree? There is a unique such choice, and it is called *Gauss–Hermite quadrature (GH)*, integrating (1) exactly whenever f is a polynomial of degree $\le 2n - 1$.

For example, for $f(x) = e^x$, the integral is $I = e^{1/4}\pi^{1/2} \approx 2.275875794469$. With just $n = 9$, GH gives the approximation $I_n \approx 2.275875794454$, accurate to better than 10^{-10}.

But the story changes for a more complicated function like $f(x) = \cos(x^3)$. To get $|I - I_n| < 10^{-10}$ with GH now, we need $n \ge 606$. Yet this integral is not really as hard as that, for although $\cos(x^3)$ wiggles a lot, the factor $\exp(-x^2)$ damps it down. In fact, if we chop the interval to $[-5, 5]$ and apply ordinary Gauss(-Legendre) quadrature, $n \ge 89$ is enough to give ten digits.

Figure 1 shows this effect for varying n. The nodes of GH span a range of order $\exp(Cn^{1/2})$. This is so wide that if f is a bounded analytic function on the real line, the outer samples contribute negligibly to (2), and the accuracy is only $O(\exp(-Cn^{1/2}))$. (With $n = 606$, 476 of the weights are below the standard machine precision of $\approx 10^{-16}$!) By contrast if we apply Gauss–Legendre quadrature on a narrower interval of size $\exp(Cn^{1/3})$, the accuracy improves to $O(\exp(-Cn^{2/3}))$.

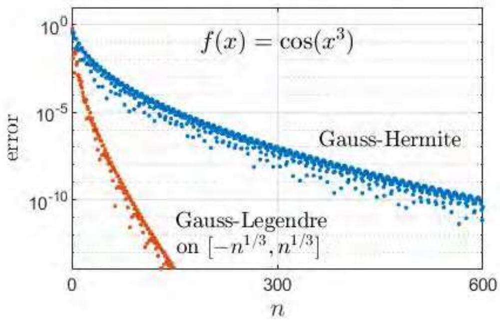

Figure 1. Gauss–Hermite quadrature, notwithstanding its optimality, converges far more slowly than chopping the real axis to a finite interval and applying a simpler formula.

How can an optimal formula be so far from optimal? The explanation is that polynomial exactness implies very little about accuracy. Polynomials must grow as $|x| \to \infty$, and loosely speaking, a formula that treats them exactly wastes most of its effort managing that growth.

We mathematicians have a way of proving theorems that are literally true, yet miss the point — I call them "inverse Yogiisms". GH is 140 years old, but although many theorems have been published, its optimality has rarely been questioned.

FURTHER READING

[1] L. N. Trefethen, Inverse Yogiisms, *Notices of the AMS*, December 2016.
[2] L. N. Trefethen, Exactness of quadrature formulas, *SIAM Review*, to appear.

Nick Trefethen
Trefethen is Professor of Numerical Analysis and head of the Numerical Analysis Group at the University of Oxford.