Experimental Mathematics

Use numerical approximation to lead us to a conjecture about a closed-form expression for a function given by an integral.

The Wikipedia entry for "Experimental mathematics" quotes Paul Halmos: "Mathematics is not a deductive science — that's a cliché. When you try to prove a theorem, you don't just list the hypotheses, and then start to reason. What you do is trial and error, experimentation, guesswork. You want to find out what the facts are, and what you do is in that respect similar to what a laboratory technician does."

For an example problem, consider this function (from the American Mathematical Monthly, March, 2003). Find a simpler formula for this function, given by a complicated integral:

$$f(x) = \int_0^{\pi/2} \operatorname{erf}(x\,\cos\theta)\,\operatorname{erf}(x\,\sin\theta)\;\sin(2\theta)\;d\theta$$

The "error function" erf is found on screen 3 of the calculator, so we can evaluate this integral for any x to look for clues about a simpler form.

Calc-50 does not do symbolic computation, so we will try to guess the formula for $f(x)$ based on numerical calculations. One approach is to compute $f(x)$ for a small x. That might give hints about any series expression for the function.

Define f1(x) to evaluate the integral for a given x. Store x in register 1 and then integrate function f2(θ) from 0 to $\pi/2$.

f1: 1, sto, 0, π, 2, /, 2, $\int_a^b$

The input to f2 is θ (saved in register 2) and the value of x in register 1 is also used to compute the integrand.

f2: 2, sto, 1, func, cos, 1, rcl, *, 3, func, erf, 1, func, 2, rcl, sin, 1, rcl, *, 3, func, erf, *,
1, func, 2, rcl, 2, *, sin, *

Like we did in the "Arctangent sum" page, we guess that $f(x)$ has a series form. This series should converge for x near zero, so we evaluate f1 at a small x (10^{-5}) and try to find a pattern in the coefficients.

$$f(x) = c_0 + c_1\,x + c_2\,x^2 + \cdots$$

40, fix, e−5, enter, 1, f_n	0.0000000000499999999983333333333750000000

This is close to $0.5 * 10^{-10}$, so we guess $c_0 = 0$, $c_1 = 0$, $c_2 = 1/2$. Multiply by 10^{10} and subtract 0.5.

e10, *, 0.5, -	−0.0000000000166666666662500000000083333333

This is close to $(-1/6) * 10^{-10}$, so we guess $c_3 = 0$, $c_4 = -1/6$. Multiply by 10^{10} and add 1/6.

e10, *, 1, enter, 6, /, +	0.0000000000041666666665833333333334722222

Multiplying this by 10^{10} gives 0.0416666666658333..., which is not quite as recognizable as a fraction, but we can check the rational approximation key, rat, on screen 2. Asking for a rational approximation with no more that 5 digits in the top and bottom gives 1/24 as a good approximation to this value. Now we think $c_5 = 0$, $c_6 = 1/24$.

e10, *, 1, enter, 24, /, −	−0.0000000000008333333333194444444446428571

Multiplying this by 10^{10} gives -0.00833333333319444..., which the rat key says is close to $-1/120$, with $c_7 = 0$, $c_8 = -1/120$.

The pattern for the even subscripts looks like alternating signs with factorials in the denominator starting with c_2:

$1/2,\ -1/6,\ 1/24,\ -1/120 = 1/2!,\ -1/3!,\ 1/4!,\ -1/5!$

This suggests

$$f(x) = \frac{1}{2!}\,x^2 - \frac{1}{3!}\,x^4 + \frac{1}{4!}\,x^6 - \frac{1}{5!}\,x^8 \cdots$$

We would like to check a few more terms to see if this pattern continues. We might get one or two more coefficients by continuing this process, but the denominators are getting bigger rapidly and cancellation error will soon win out. But if we hadn't thought of it earlier, these factorials might suggest using the definition of the Maclaurin series directly.

$$f(x) = f(0) + \frac{f'(0)}{1!}\,x + \frac{f''(0)}{2!}\,x^2 + \frac{f'''(0)}{3!}\,x^3 + \cdots$$

The n$^{\text{th}}$ derivative key on screen 6 can compute these derivatives more accurately, but it will be a bit slow since we are computing numerical derivatives of a function defined in terms of a numerical integral.

Define f3(n) to evaluate $f^{(n)}(0)/n!$.

f3: 3, sto, 0, x↔y, 1, f$^{(\text{n})}$, 3, func, 3, rcl, x!, /

0, enter, 3, f_n	0.0000000000000000000000000000000000000000
1, enter, 3, f_n	0.0000000000000000000000000000000000000000
2, enter, 3, f_n	0.5000000000000000000000000000000000000000
3, enter, 3, f_n	0.0000000000000000000000000000000000000000
4, enter, 3, f_n	−0.1666666666666666666666666666666666666667
5, enter, 3, f_n	0.0000000000000000000000000000000000000000
6, enter, 3, f_n	0.0416666666666666666666666666666666666667
7, enter, 3, f_n	0.0000000000000000000000000000000000000000
8, enter, 3, f_n	−0.0083333333333333333333333333333333333333
10, enter, 3, f_n	0.0013888888888888888888888888888888888889
12, enter, 3, f_n	−0.0001984126984126984126984126984126984127
14, enter, 3, f_n	0.0000248015873015873015873015873015873016

These even terms agree with reciprocals of factorials out to 1/8! for $n = 14$. That makes the conjectured series for $f(x)$ seem more likely to be true. Since the terms in this series are not very complicated, maybe we can relate it to a known function. The factorials in the denominators remind us of the exponential function, so start there and try to turn it into our series.

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \frac{x^5}{5!} + \cdots$$

$$\Rightarrow \quad e^{-x^2} = 1 - \frac{x^2}{1!} + \frac{x^4}{2!} - \frac{x^6}{3!} + \frac{x^8}{4!} - \frac{x^{10}}{5!} + \cdots$$

$$\Rightarrow \quad e^{-x^2} - 1 + x^2 = \frac{x^4}{2!} - \frac{x^6}{3!} + \frac{x^8}{4!} - \frac{x^{10}}{5!} + \cdots$$

$$\Rightarrow \quad \frac{e^{-x^2} - 1 + x^2}{x^2} = \frac{x^2}{2!} - \frac{x^4}{3!} + \frac{x^6}{4!} - \frac{x^8}{5!} + \cdots$$

This last series agrees with our series for $f(x)$ so now we have a conjecture for the closed form of the original integral.

$$f(x) = \int_0^{\pi/2} \operatorname{erf}(x \cos\theta) \operatorname{erf}(x \sin\theta) \ \sin(2\theta) \ d\theta = \frac{e^{-x^2} - 1 + x^2}{x^2}$$

With some confidence that this last equation is true, the numerical and experimental part of the analysis is done. Knowing the answer often makes the mathematical proof of the result easier to find. Sometimes there are even clues in the number-crunching part of the process that can help with the final proof. Since our interest here is with the numerical calculations, we will leave the actual proof as an exercise for the reader.