

NUMERICAL INTEGRATION

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In my first year at university, our lecturer offered a \$100 prize to anyone who could work out

$$\int e^{-x^2} dx$$

in terms of so-called elementary functions, (i.e. polynomials, rational functions, exponential, trigonometric or logarithmic functions). Needless to say, he didn't have to part with his \$100 since the problem cannot be solved. An approximate value can, however, be obtained to

$$\int_a^b e^{-x^2} dx$$

for given a and b using a numerical approximation formula such as the Trapezoidal Rule or Simpson's rule which you will study (or have studied) at school. The famous mathematician Gauss (1777 - 1855) gave a rather nice and very practical technique for finding the approximate value of a definite integral.

Suppose, firstly, we wish to evaluate $\int_{-1}^1 f(x) dx$, where $f(x)$ is a given function. The approximation is given by

$$\int_{-1}^1 f(x) \approx af(\alpha) + bf(\beta)$$

where a, α, b, β are chosen such that we can replace \approx by $=$ for the functions $f(x) = 1, x, x^2, x^3$.

Substituting we obtain

$$\begin{aligned} \int_{-1}^1 1 dx = 2 &\Rightarrow a + b = 2 \\ \int_{-1}^1 x dx = 0 &\Rightarrow a\alpha + b\beta = 0 \\ \int_{-1}^1 x^2 dx = \frac{2}{3} &\Rightarrow a\alpha^2 + b\beta^2 = \frac{2}{3} \\ \text{and } \int_{-1}^1 x^3 dx = 0 &\Rightarrow a\alpha^3 + b\beta^3 = 0. \end{aligned}$$

These four non-linear equations in four unknowns can be solved to give $a = b = 1$, $\alpha = -\beta$ and $\alpha^2 = \frac{1}{3}$.

Hence the formula becomes

$$\int_{-1}^1 f(x) dx \approx f\left(\frac{1}{\sqrt{3}}\right) + f\left(-\frac{1}{\sqrt{3}}\right)$$

and this formula will be **exact** for all cubic functions.

Applying the formula to

$$\int_{-1}^1 (2x^3 + 3x^2 - x + 1) dx$$

gives 4 which is the exact value obtained by integration. (My calculator in fact gives 4.000000006 because of the rounding error involved in the approximation of $\frac{1}{\sqrt{3}}$).

It may at first appear that the formula is limited to definite integrals between -1 and 1 , but a change of variable gives a more general form.

If you make the substitution $x = \frac{1}{2}[(b-a)u + (a+b)]$ in the integral $\int_a^b f(x)dx$, then $x = a$ gives $u = -1$ and $x = b$ gives $u = 1$ and $dx = \frac{1}{2}(b-a)du$, so

$$\int_a^b f(x)dx = \left(\frac{b-a}{2}\right) \int_{-1}^1 f\left(\frac{1}{2}[(b-a)u + (a+b)]\right) du.$$

An example will illustrate how this works.

If $I = \int_3^4 \frac{1}{\ln x} dx$, let $x = \frac{1}{2}(u+7)$, then $I = \frac{1}{2} \int_{-1}^1 \frac{1}{\ln\left(\frac{u+7}{2}\right)} du$, so $f(u) = \frac{1}{\ln\left(\frac{u+7}{2}\right)}$.

Applying the formula we have

$$\begin{aligned} I &\approx \frac{1}{2} \left[f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \right] \\ &= \frac{1}{2} \left[\frac{1}{\ln\frac{1}{2}\left(7 - \frac{1}{\sqrt{3}}\right)} + \frac{1}{\ln\frac{1}{2}\left(7 + \frac{1}{\sqrt{3}}\right)} \right] \simeq 0.803936 \end{aligned}$$

A more exact value is 0.803996499, however the formula is still fairly accurate.

To find an approximate value of $I = \int_0^{\frac{\pi}{2}} \sin x dx$, put

$$x = \frac{1}{2} \left[\frac{\pi}{2} u + \frac{\pi}{2} \right] = \frac{\pi}{4}(u+1), \text{ then } I = \frac{\pi}{4} \int_{-1}^1 \sin \frac{\pi}{4}(u+1) du$$

and the formula gives 0.99848. (The exact value is of course 1).

Gauss' formula can be improved by taking 4 function values and writing

$$\int_{-1}^1 f(x)dx \approx a_1 f(\alpha_1) + a_2 f(\alpha_2) + a_3 f(\alpha_3) + a_4 f(\alpha_4)$$

where the unknowns are determined by replacing \approx by $=$ for $f(x) = 1, x, x^2, \dots, x^7$. Unfortunately the 8 non-linear equations in 8 unknowns are difficult to solve by hand. Using a computer I obtained

$$\begin{aligned} \int_{-1}^1 f(x)dx \approx & 0.347855845[f(-0.861136312) + f(0.861136312)] \\ & + 0.652145155[f(-0.339981044) + f(0.339981044)] \end{aligned}$$

which will be exact (save for rounding error) for all polynomials of degree less or equal to 7.

[In fact, the exact formula is

$$\begin{aligned} \left(\frac{1}{2} - \frac{\sqrt{30}}{36}\right) & \left[f\left(-\sqrt{\frac{30 + \sqrt{480}}{70}}\right) + f\left(\sqrt{\frac{30 + \sqrt{480}}{70}}\right) \right] \\ & + \left(\frac{1}{2} + \frac{\sqrt{30}}{36}\right) \left[f\left(-\sqrt{\frac{30 - \sqrt{480}}{70}}\right) + f\left(\sqrt{\frac{30 - \sqrt{480}}{70}}\right) \right] \end{aligned}$$

You should write out the 8 equations and verify that these numbers are in fact solutions.

To test it out, I approximated $\int_0^{\frac{\pi}{2}} \sin x \, dx$ and obtained 0.9999999773 on my calculator.

You might like to try Simpson's rule on this integral and see how many strips you need to obtain the same accuracy.

Although the four point formula seems difficult to calculate with (and certainly impossible to remember!), it is very easy to program into your home computer.

Try using the four point formula to get an approximate value of $\int_0^1 e^{-x^2} dx$.