Quadrature

As previously noted, this is the 'fancy' NA term for [definite] integration. In the simple cases, we are working out an integral such as $\int_a^b f(x)\,\mathrm{d}x$, where f is some given function. In more advanced work, we would look at various sorts of 'improper' integral, such as those where either or both limit is infinite, and at integrals with a 'weight' function, such as $\int_0^\infty f(x)\,\mathrm{e}^{-x}\,\mathrm{d}x$. We would also be looking at multiple integrals, contour integrals, surface integrals, and so on.

All of the standard methods rely basically on approximating f by a polynomial, and integrating that instead of f. Ideally, the approximation has low degree—quadratic or cubic, occasionally quartic. Do not be tempted to use high-degree polynomials; these are almost always very unstable, and good results depend on f being extremely well-behaved.

Never try to use quadrature on functions that are not well-behaved. If f does not 'look like' a polynomial, then integrating it as though it does is simply not going to work. Not never, not nohow.

Anyway, this motivates us to study first how to approximate functions by polynomials. This will give us an 'interpolating' polynomial, which can be used to 'replace' f in suitable numerical processes.

Interpolation

This is a *major* subject in its own right. We can try to fit a polynomial [or other function, in general] to *(a)* a function and its derivatives at a point; *(b)* a set of data points; or *(c)* some known function [and perhaps its derivatives] over a range of x-values. Case *(a)* is about the Taylor series of f, and is not relevant to this module. Case *(c)* is also an exercise in calculus; it *is* relevant, but we're not going to do it here.

So we concentrate on *(b)*, the problem of fitting a curve to some data points. Note that this is closely related to methods such as 'least squares' for fitting lines or curves to experimental data. Again, there are lots of possible criteria for the polynomial. We can try to make the curve go through some or all of the points; we can try to make it run as close as possible to some or all of the points; 'as close as possible' could be interpreted as lowest sum of squared error ['least squares'], or as minimised maximum deviation, or in various other ways. In this module, we look only at the problem of making a low-degree polynomial go through certain points.

To fix ideas, let us look at the Wallis polynomial again:

x	0	1	2	3	4
$W(x)$	–5	–6	–1	16	51

There are two basic ways to proceed; they give the same answer, so you can choose which you prefer.

Firstly, note that, for example, the polynomial

$$(x-0)(x-1)(x-2)(x-4)$$

[No $(x-3)$!] is, by construction, zero when x is 0, 1, 2 or 4. When $x = 3$, it has the value

$$(3-0)(3-1)(3-2)(3-4) = -6.$$

So the [quartic, in this case] polynomial

$$-16\,(x-0)(x-1)(x-2)(x-4)\,/\,6 = -\tfrac{8}{3}x^4 + \tfrac{56}{3}x^3 - \tfrac{112}{3}x^2 + \tfrac{64}{3}x$$

has the right value of $W(3)$ when $x = 3$ and is zero at the other given data points. If we write down the corresponding [quartic] polynomials for the other four data points, and add up all five polynomials, then at each data point four or them will be zero and the fifth will have the right value; so it will have the right value in total. *Exercise:* do this [perhaps using Maple!] and verify that you get the Wallis cubic out of it!

The second way works by interpolating a few points at a time and combining them. For example, the interpolating *quadratic* for $x = 0$, 1, 2 is $3x^2 - 4x - 5$, while that for $x = 1, 2, 3$ is $6x^2 - 13x + 1$ [left as an exercise!]. So to get the interpolating *cubic* for $x = 0, 1, 2, 3$, we have to 'fade out' the first quadratic and 'fade in' the second as x changes from 0 to 3. The fading out is done by multiplying the first quadratic by $(3-x)/3$ [which is 1 when $x = 0$ and 0 when $x = 3$]; and the fading in by multiplying the second quadratic by $(x-0)/3$ [which is 0 when $x = 0$ and 1 when $x = 3$]. So the interpolating cubic is

$$\tfrac{1}{3}(3-x)(3x^2 - 4x - 5) + \tfrac{1}{3}(x-0)(6x^2 - 13x + 1) = x^3 - 2x - 5$$

[now *there's* a surprise!]. We start the process off with the 'interpolating constants', -5, -6 and so on that are each right at one data point; we fade them in and out to get the interpolating linear 'curves' between adjacent pairs of points; fade them in and out to get quadratics between triples, then cubics, quartics and so on.

The total work done will be the same in both methods; but the second method gives useful lower-order polynomials for parts of the function as the higher ones are built up. You can save yourself lots of hard work by using Maple; see the *interp* command [the help for which will direct you to 'more modern' equivalents, and to lots of other interpolation techniques].

Note that, for example, the interpolating cubic for

x	0	0.1	0.2	0.3
$\sin x$	0.0000000000	0.0998334166	0.1986693308	0.2955202067

is, according to Maple,

$$1.000029893\,x - 0.00049833998\,x^2 - 0.1645892834\,x^3,$$

which is somewhat different from the Taylor series, $x - \frac{1}{6}x^3$ to the same degree. But the interpolated polynomial gives $\sin 0.25 \approx 0.2474046194$, which is much nearer the actual value of 0.2474039593 than the Taylor series, which gives 0.2473958333.

Interpolating quadratics, and Simpson's Rule

The most useful interpolation for quadrature is the quadratic through three equally-spaced points. Essentially, what Simpson did was to go through the above process, but in full generality; then he integrated the result. The algebra is done once, then we can re-use and re-use it indefinitely.

Specifically, suppose we are integrating between a and b; that $c = \frac{1}{2}(a+b)$ is the mid-point between a and b; and that $c-a = b-c = h$. Then we have the table:

x	$a = c-h$	c	$b = c+h$
$f(x)$	$f(a)$	$f(c)$	$f(b)$

with interpolating quadratic ..., well, something quite messy:

$$\tfrac{1}{2} h^{-2}([f(a)+f(b)-2f(c)](x-c)^2 - h[f(a)-f(b)](x-c) + 2h^2 f(c))$$

[left in terms of h and $x-c$ for 'symmetry']. Now we need to integrate that for x between $c-h$ and $c+h$; but we only need to do it once, and it is only a quadratic. The result [you can use Maple!] is

$$\int_a^b f(x)\,\mathrm{d}x \approx \tfrac{1}{3} h\,(f(a)+4f(c)+f(b)),$$

our old friendly neighbourhood Simpson's Rule.