§3 Numerical Integration

§3.4 Gaussian Quadrature

MA378 – Numerical Analysis II ("NA2")

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This section is perhaps the most mathematically rich in the course. I'd encourage you to read further: Chapter 10 of Süli and Mayers is devoted to this. However, much of the basic theory is developed in Section 9.4 on Orthogonal Polynomials. See also Lectures 22 and 23 of Stewart's "Afternotes goes to Grad School".

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To date we have found some numerical schemes that approximate $\int_a^b f(x)dx$ as the weighted average of values of f at $n+1$ equally spaced points. These methods have precision n (or $n+1$ in special cases).

With Gaussian Quadrature we choose both the quadrature weights *and points* in such as way as to maximize the precision of the method.

There are three equivalent approaches to finding these points and weights that maximize the precision.

(i) ***Undetermined Coefficients***: The obvious way for, say, $n = 2$. But, unlike Newton-Cotes, we have to solve a system of *nonlinear* equations. Even for $n = 3$ this can become difficult.

(ii) Base the method on integrating the ***Hermite Interpolant*** of the integrand, f, and choose the points so that the coefficients of $f'(x_i)$ are zero. This approach is the easiest to analyse, but less useful for construction.

(iii) ***Finding the zeros of the members of a sequence of orthogonal monic polynomials***. This is the approach we will emphasise most, as it gives us an easy way of proving the precision of the methods.

Example

Find a two point rule

$$\int_{-1}^{1} f(x)dx \approx G_1(f) := w_0 f(x_0) + w_1 f(x_1),$$

that is exact for all polynomials of degree 3 or less.

This leads a the non-linear system which we must solve for w_0, x_0, w_1, x_1. This has $\underline{\underline{4}}$ degrees of freedom. So the method can be made to be exact for polynomials of degree 0, eg $p_0 \equiv 1$, degree 1, eg $p_1 = x$, degree 2, eg $p_2(x) = x^2$, & 3 eg $p_3 = x^3$.

Example

Find a two point rule

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that is exact for all polynomials of degree 3 or less.

This leads a the non-linear system which we must solve: the following equations

$f(x) = 1$ $\quad G_1(1) = \int_{-1}^{1} 1\,dx \Rightarrow \quad w_0 + w_1 = 2$

$f(x) = x$ $\quad G_1(x) = \int_{-1}^{1} x\,dx \Rightarrow \quad w_0 x_0 + w_1 x_1 = 0$

$f(x) = x^2$ $\quad G_1(x^2) = \int_{-1}^{1} x^2\,dx \Rightarrow \quad w_0 x_0^2 + w_1 x_1^2 = 2/3$

$f(x) = x^3$ $\quad G_1(x^3) = \int_{-1}^{1} x^3\,dx \Rightarrow \quad w_0 x_0^3 + w_1 x_1^3 = 0$

(1) $w_0 + w_1 = 2$

(2) $w_0 x_0 + w_1 x_1 = 0$

(3) $w_0 x_0^2 + w_1 x_1^2 = 2/3$

(4) $w_0 x_0^3 + w_1 x_1^3 = 0$

From (2) $w_0 x_0 = -w_1 x_1$

Sub into (4) to get

$(w_0 x_0) x_0^2 + w_1 x_1^3 = 0$

$\Rightarrow -w_1 x_1 x_0^2 + w_1 x_1^3 = 0$

None of the w_i are zero, so dividing by w_1 gives $-x_1 x_0^2 + x_1^3 = 0$. Next, $x_1 \neq 0$ otherwise $x_0 = 0$ too, but $x_0 \neq x_1$. So now $x_0^2 = x_1^2$. That is $x_0 = -x_1$.

See board.

That is

$$\int_{-1}^{1} f(x)dx \approx G_1(f) := f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right). \qquad (1)$$

Example

Let $f(x) = \exp(-x)$.
If we estimate $\int_{-1}^{1} f(x)dx$ using each of

(a) ***Trapezium Rule***,

(b) ***Simpson's Rule*** and

(c) the ***Gaussian Rule*** above

we find the errors are, respectively, 0.735, 0.01165 and 0.00771.
Using the ***composite Trapezium rule***, we find we would have to take $N = 11$ to obtain an estimate that is more accurate than the two-point Gaussian Rule.

Note that the Trap Rule & G_1 both require 2 function evaluations, but the difference in Error is about a factor of 100.

Example

If you use the $G_1(\cdot)$ rule to estimate $\int_0^{\pi/4} \cos(x)dx$ you'll get

$$G_1(\cos) = 0.07070432596.$$

$x_1 = ?$

$x_2 = ?$

Computing the exact error, we find that

$$\Big|\int_0^{\pi/4} \cos(x)dx - G_1(\cos)\Big| = \Big|\frac{1}{\sqrt{2}} - 0.07070432596\Big| \approx 6.35 \times 10^{-5}.$$

Compare with results for the same problem when

- The Trapezium rule is used. ~ 0.039
- Simpson's rule is used. $\sim 5.? \times 10^{-4}$.

Example (3-point Gauss-Lobatto method)

The ***Gauss-Lobatto method*** is a variation on Gaussian quadrature.
Rather than allowing all of the quadrature points to vary in order to maximize the precision of the method, we fix some of them — usually the end points.
Use undetermined coefficients to derive the 3-point rule:

$$\int_{-1}^{1} f(x)dx \approx w_0 f(\mathbf{-1}) + w_1 f(x_1) + w_2 f(1).$$

note that this has 4 degrees of freedom : w_0, w_1, w_2 & x_1. So should be exact for 1, x, x^2, x^3.

(see board). The 4 equations are

$$w_0 + w_1 + w_2 = 2 \quad (i)$$
$$-w_0 + w_1 x_1 + w_2 = 0 \quad (ii)$$
$$w_0 + w_1 x_1^2 + w_2 = 2/3 \quad (iii)$$
$$-w_0 + w_1 x_1^3 + w_2 = 0. \quad (iv).$$

Subtraction (iv) from (ii) gives

$w_1 (x_1 - x_1^3) = 0 \Rightarrow x_1 - x_1^3 = 0 \quad (w_1 \neq 0)$

$\Rightarrow x_1 (1 - x_1^2) = 0$. So, either $x_1 = 0$ (Ok)

or $x_1^2 = 1$ (no ok: $x_1 \neq -1$, $x_1 \neq 1$).

With a little work get $w_0 = 1/3$, $w_1 = 4/3$, $w_2 = 1/3$

SIMPSON's Rule again!