MA378 Chapter 3: Numerical Integration

§3.4 Gaussian Quadrature

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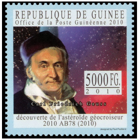

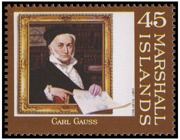

Johann Carl Friedrich Gauß, born 1777 in Braunschweig, died 1855 in Göttingen

4.1 Gaussian Quadrature

Sections 3.4, 3.5 and 3.6 are, 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".

. . . .

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.

4.1 Gaussian Quadrature

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

(i) **Undetermined Coefficients**: This is the obvious way to derive the methods for, say, $N = 2$. But, unlike Newton-Cotes, we have to solve a system of *nonlinear* equations. For larger N 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.

 Note we use w_i for weights.

Example 4.1

Find a two point rule

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

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

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

We have 4 unknowns w_0, w_1, x_0 & x_1

So we need to solve 4 equations:

$$G_1(1) = \int_{-1}^{1} 1\,dx \qquad G_1(x) = \int_{-1}^{1} x\,dx$$

$$G_1(x^2) = \int_{-1}^{1} x^2\,dx \qquad G_1(x^3) = \int_{-1}^{1} x^3\,dx$$

Try this! [Finish here Friday 1/3/24]

4.2 Undetermined Coefficients

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

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

(iii) $f(x) = x^2 \Rightarrow \quad \Rightarrow w_0 x_0^2 + w_1 x_1^2 = 2/3$

(iv) $f(x) = x^3 \Rightarrow \quad \Rightarrow w_0 x_0^3 + w_1 x_1^3 = 0$

(ii) $\Rightarrow w_0 x_0 = -w_1 x_1$

(iv): $w_0 x_0^3 = -w_1 x_1^3 \Rightarrow w_0 x_0^3 = (-w_1 x_1) x_1^2$

$\Rightarrow w_0 x_0^3 = w_0 x_0 x_1^2$

That is $\Rightarrow x_0^3 = x_0 x_1^2$ since $w_0 \neq 0$.

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

4.2 Undetermined Coefficients

So we have $x_0^3 = x_0 x_1^2$.

If $x_0 \neq 0$ then $x_0^2 = x_1^2$. So $x_0 = -x_1$

[Exer: show there is no solution if $x_0 = 0$].

That is

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

Now use (say) Eqn (ii) again

$w_0 x_0 + w_1 x_1 = 0 \implies w_0 x_0 - w_1 x_0 = 0.$

$\implies w_0 = w_1$ since $x_0 \neq 0$.

Then apply (i) to get

$w_0 + w_1 = 2 \implies \boxed{w_0 = w_1 = 1.}$

Finally apply (iii) to get

$w_0 x_0^2 + w_1 x_1^2 = 2/3 \implies x_0^2 + x_1^2 = 2/3 \implies 2x_0^2 = 2$

$\implies \boxed{x_0 = -1/\sqrt{3}.}$. Also $\boxed{x_1 = 1/\sqrt{3}}$

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 4.2

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

(a) **Trapezium Rule**, we get error of 0.735

(b) **Simpson's Rule**: error is 0.01165

(c) the 2-point **Gaussian Rule**: error is 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: Do Exer 4.1]

Example 4.3

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

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

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.
- Simpson's rule is used.

Example 4.4 (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:

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

That is: we set $x_0=-1$, $x_2=1$, and find x_1, w_0, w_1 and w_2 to optimise the precision of the Rule. This should be Exact for $f(x)=1$, $f(x)=x$, $f(x)=x^2$, $f(x)=x^3$.

 Simpson's Rule Again!!

Each of these gives an equation.
(See board!)

Solving them gives . . .
(after some work)

$x_1 = 0$,

$w_0 = 1/3$, $w_1 = 4/3$, $w_2 = 1/3$.

So the Method is

$$\int_{-1}^{1} f(x)\,dx \overset{?}{=} \frac{1}{3}\Big(f(-1) + 4f(0) + f(1)\Big),$$

4.3 Exercises

Idea: find $g(x)$ that maps $[-1,1]$ to $[a,b]$.

Exercise 4.1

Use a change of variables, as we did with the Trapezium rule, to show that the rule for approximating $\int_0^1 f(x)dx$ is

$\hookrightarrow$ Then new points are $g(x_0), g(x_1)$ and weights are $\dfrac{dg}{dx}$

$$G_1(f) = \frac{1}{2}\Big(f(\frac{1}{2} - \frac{1}{2\sqrt{3}}) + f(\frac{1}{2} + \frac{1}{2\sqrt{3}})\Big).$$

More generally, extend the $G_1(f)$ rule in (1) to an arbitrary interval $[a, b]$.

Exercise 4.2

Use $G_1(x)$ to estimate $\int_1^2 \ln(x)dx$. How does this compare with the Trapezium and Simpson's Rule?

Exercise 4.3 (Assignment)

Derive a 3-point Gaussian Quadrature Rule to estimate $\int_{-1}^1 f(x)dx$. *Hint:* $x_1 = 0$.