NUMERICAL INTEGRATION: ANOTHER APPROACH

We look for numerical integration formulas

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{j=1}^{n} w_j f(x_j)$$

which are to be **exact** for polynomials of as large a degree as possible. There are no restrictions placed on the nodes $\left\{x_j\right\}$ nor the weights $\left\{w_j\right\}$ in working towards that goal. The motivation is that if it is exact for high degree polynomials, then perhaps it will be very accurate when integrating functions that are well approximated by polynomials.

There is no guarantee that such an approach will work. In fact, it turns out to be a bad idea when the node points $\left\{x_j\right\}$ are required to be evenly spaced over the interval of integration. But without this restriction on $\left\{x_j\right\}$ we are able to develop a very accurate set of quadrature formulas.

The case $n = 1$. We want a formula

$$w_1 f(x_1) \approx \int_{-1}^{1} f(x)\, dx$$

The weight w_1 and the node x_1 are to be so chosen that the formula is exact for polynomials of as large a degree as possible.

To do this we substitute $f(x) = 1$ and $f(x) = x$. The first choice leads to

$$\begin{aligned} w_1 \cdot 1 &= \int_{-1}^{1} 1\, dx \\ w_1 &= 2 \end{aligned}$$

The choice $f(x) = x$ leads to

$$\begin{aligned} w_1 x_1 &= \int_{-1}^{1} x\, dx = 0 \\ x_1 &= 0 \end{aligned}$$

The desired formula is

$$\int_{-1}^{1} f(x)\, dx \approx 2f(0)$$

It is called the *midpoint rule* and was introduced in the problems of Section 5.1.

The case $n = 2$. We want a formula

$$w_1 f(x_1) + w_2 f(x_2) \approx \int_{-1}^{1} f(x)\,dx$$

The weights w_1, w_2 and the nodes x_1, x_2 are to be so chosen that the formula is exact for polynomials of as large a degree as possible. We substitute and force equality for

$$f(x) = 1, x, x^2, x^3$$

This leads to the system

$$\begin{aligned} w_1 + w_2 &= \int_{-1}^{1} 1\,dx = 2 \\ w_1 x_1 + w_2 x_2 &= \int_{-1}^{1} x\,dx = 0 \\ w_1 x_1^2 + w_2 x_2^2 &= \int_{-1}^{1} x^2\,dx = \frac{2}{3} \\ w_1 x_1^3 + w_2 x_2^3 &= \int_{-1}^{1} x^3\,dx = 0 \end{aligned}$$

The solution is given by

$$w_1 = w_2 = 1, \quad x_1 = \frac{-1}{\mathrm{sqrt}(3)}, \quad x_2 = \frac{1}{\mathrm{sqrt}(3)}$$

This yields the formula

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

We say it has *degree of precision* equal to 3 since it integrates exactly all polynomials of degree ≤ 3. We can verify directly that it does not integrate exactly $f(x) = x^4$.

$$\int_{-1}^{1} x^4\,dx = \tfrac{2}{5}$$

$$f\left(\frac{-1}{\mathsf{sqrt}(3)}\right) + f\left(\frac{1}{\mathsf{sqrt}(3)}\right) = \tfrac{2}{9}$$

Thus (1) has degree of precision exactly 3.

EXAMPLE Integrate

$$\int_{-1}^{1} \frac{dx}{3+x} = \log 2 \doteq 0.69314718$$

The formula (1) yields

$$\frac{1}{3+x_1} + \frac{1}{3+x_2} = 0.69230769$$

$$Error = .000839$$

THE GENERAL CASE

We want to find the weights $\{w_i\}$ and nodes $\{x_i\}$ so as to have

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{j=1}^{n} w_j f(x_j)$$

be exact for a polynomials $f(x)$ of as large a degree as possible. As unknowns, there are n weights w_i and n nodes x_i. Thus it makes sense to initially impose $2n$ conditions so as to obtain $2n$ equations for the $2n$ unknowns. We require the quadrature formula to be exact for the cases

$$f(x) = x^i, \qquad i = 0, 1, 2, ..., 2n-1$$

Then we obtain the system of equations

$$w_1 x_1^i + w_2 x_2^i + \cdots + w_n x_n^i = \int_{-1}^{1} x^i\,dx$$

for $i = 0, 1, 2, ..., 2n-1$. For the right sides,

$$\int_{-1}^{1} x^i\,dx = \begin{cases} \dfrac{2}{i+1}, & i = 0, 2, ..., 2n-2 \\ 0, & i = 1, 3, ..., 2n-1 \end{cases}$$

The system of equations

$$w_1 x_1^i + \cdots + w_n x_n^i = \int_{-1}^{1} x^i \, dx, \quad i = 0, ..., 2n-1$$

has a solution, and the solution is unique except for re-ordering the unknowns. The resulting numerical integration rule is called *Gaussian quadrature*.

In fact, the nodes and weights are not found by solving this system. Rather, the nodes and weights have other properties which enable them to be found more easily by other methods. There are programs to produce them; and most subroutine libraries have either a program to produce them or tables of them for commonly used cases.

SYMMETRY OF FORMULA

The nodes and weights possess symmetry properties. In particular,

$$x_i = -x_{n-i}, \qquad w_i = w_{n-i}, \qquad i = 1, 2, ..., n$$

A table of these nodes and weights for $n = 2, ..., 8$ is given in the text in Table 5.7. A *MATLAB* program to give the nodes and weights for an arbitrary finite interval $[a, b]$ is given in the class account.

In addition, it can be shown that all weights satisfy

$$w_i > 0$$

for all $n > 0$. This is considered a very desirable property from a practical point of view. Moreover, it permits us to develop a useful error formula.

CHANGE OF INTERVAL OF INTEGRATION

Integrals on other finite intervals $[a, b]$ can be converted to integrals over $[-1, 1]$, as follows:

$$\int_a^b F(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} F\left(\frac{b+a+t(b-a)}{2}\right)dt$$

based on the change of integration variables

$$x = \frac{b+a+t(b-a)}{2}, \qquad -1 \le t \le 1$$

EXAMPLE Over the interval $[0, \pi]$, use

$$x = (1+t)\,\tfrac{\pi}{2}$$

Then

$$\int_0^{\pi} F(x)\ dx = \tfrac{\pi}{2}\int_{-1}^{1} F\left((1+t)\,\tfrac{\pi}{2}\right)\ dt$$

EXAMPLE Consider again the integrals used as examples in Section 5.1:

$$\begin{aligned} I^{(1)} &= \int_0^1 e^{-x^2} dx \doteq .74682413281234 \\ I^{(2)} &= \int_0^4 \frac{dx}{1+x^2} = \arctan 4 \\ I^{(3)} &= \int_0^{2\pi} \frac{dx}{2+\cos x} = \frac{2\pi}{\text{sqrt}(3)} \end{aligned}$$

n	$I - I^{(1)}$	$I - I^{(2)}$	$I - I^{(3)}$
2	$2.29E-4$	$-2.33E-2$	$8.23E-1$
3	$9.55E-6$	$-3.49E-2$	$-4.30E-1$
4	$-3.35E-7$	$-1.90E-3$	$1.77E-1$
5	$6.05E-9$	$1.70E-3$	$-8.12E-2$
6	$-7.77E-11$	$2.74E-4$	$3.55E-2$
7	$8.60E-13$	$-6.45E-5$	$-1.58E-2$
10	$*$	$1.27E-6$	$1.37E-3$
15	$*$	$7.40E-10$	$-2.33E-5$
20	$*$	$*$	$3.96E-7$

Compare these results with those of Section 5.1.

AN ERROR FORMULA

The usual error formula for Gaussian quadrature formula,

$$E_n(f) = \int_{-1}^{1} f(x)\,dx - \sum_{j=1}^{n} w_j f(x_j)$$

is not particularly intuitive. It is given by

$$\begin{aligned} E_n(f) &= e_n \frac{f^{(2n)}(c_n)}{(2n)!} \\ e_n &= \frac{2^{2n+1}\,(n!)^4}{(2n+1)\,[(2n)!]^2} \approx \frac{\pi}{4^n} \end{aligned}$$

for some $a \le c_n \le b$.

To help in understanding the implications of this error formula, introduce

$$M_k = \max_{-1 \le x \le 1} \frac{\left| f^{(k)}(x) \right|}{k!}$$

With many integrands $f(x)$, this sequence $\{M_k\}$ is bounded or even decreases to zero. For example,

$$f(x) = \begin{cases} \cos x \\ \dfrac{1}{2+x} \end{cases} \quad \Rightarrow \quad M_k \le \begin{cases} \dfrac{1}{k!} \\ 1 \end{cases}$$

Then for our error formula,

$$\begin{aligned} E_n(f) &= e_n \frac{f^{(2n)}(c_n)}{(2n)!} \\ |E_n(f)| &\le e_n M_{2n} \end{aligned} \tag{2}$$

By other methods, we can show

$$e_n \approx \frac{\pi}{4^n}$$

When combined with (2) and an assumption of uniform boundedness for $\{M_k\}$, we have the error decreases by a factor of at least 4 with each increase of n to $n+1$. Compare this to the convergence of the trapezoidal and Simpson rules for such functions, to help explain the very rapid convergence of Gaussian quadrature.

A SECOND ERROR FORMULA

Let $f(x)$ be continuous for $a \le x \le b$; let $n \ge 1$. Then, for the Gaussian numerical integration formula

$$I \equiv \int_a^b f(x)\,dx \approx \sum_{j=1}^{n} w_j f(x_j) \equiv I_n$$

on $[a, b]$, the error in I_n satisfies

$$|I(f) - I_n(f)| \le 2\,(b-a)\,\rho_{2n-1}(f) \tag{3}$$

Here $\rho_{2n-1}(f)$ is the minimax error of degree $2n-1$ for $f(x)$ on $[a, b]$:

$$\rho_m(f) = \min_{\deg(p)\le m}\left[\max_{a\le x\le b}|f(x)-p(x)|\right], \quad m \ge 0$$

EXAMPLE Let $f(x) = e^{-x^2}$. Then the minimax errors $\rho_m(f)$ are given in the following table.

m	$\rho_m(f)$	m	$\rho_m(f)$
1	5.30E − 2	6	7.82E − 6
2	1.79E − 2	7	4.62E − 7
3	6.63E − 4	8	9.64E − 8
4	4.63E − 4	9	8.05E − 9
5	1.62E − 5	10	9.16E − 10

Using this table, apply (3) to

$$I = \int_0^1 e^{-x^2}\, dx$$

For $n = 3$, (3) implies

$$|I - I_3| \leq 2\rho_5\left(e^{-x^2}\right) \doteq 3.24 \times 10^{-5}$$

The actual error is 9.55E − 6.

INTEGRATING A NON-SMOOTH INTEGRAND

Consider using Gaussian quadrature to evaluate
$I = \int_0^1 \text{sqrt}(x)\ dx = \frac{2}{3}$

n	$I - I_n$	*Ratio*
2	$-7.22\text{E}-3$	
4	$-1.16\text{E}-3$	6.2
8	$-1.69\text{E}-4$	6.9
16	$-2.30\text{E}-5$	7.4
32	$-3.00\text{E}-6$	7.6
64	$-3.84\text{E}-7$	7.8

The column labeled *Ratio* is defined by

$$\frac{I - I_{\frac{1}{2}n}}{I - I_n}$$

It is consistent with $I - I_n \approx \dfrac{c}{n^3}$, which can be proven theoretically. In comparison for the trapezoidal and Simpson rules, $I - I_n \approx \dfrac{c}{n^{1.5}}$

WEIGHTED GAUSSIAN QUADRATURE

Consider needing to evaluate integrals such as

$$\int_0^1 f(x) \log x \, dx, \qquad \int_0^1 x^{\frac{1}{3}} f(x) \, dx$$

How do we proceed? Consider numerical integration formulas

$$\int_a^b w(x) f(x) \, dx \approx \sum_{j=1}^{n} w_j f(x_j)$$

in which $f(x)$ is considered a "nice" function (one with several continuous derivatives). The function $w(x)$ is allowed to be singular, but must be integrable. We assume here that $[a, b]$ is a finite interval. The function $w(x)$ is called a "weight function", and it is implicitly absorbed into the definition of the quadrature weights $\{w_i\}$. We again determine the nodes $\{x_i\}$ and weights $\{w_i\}$ so as to make the integration formula exact for $f(x)$ a polynomial of as large a degree as possible.

The resulting numerical integration formula

$$\int_a^b w(x) f(x)\, dx \approx \sum_{j=1}^{n} w_j f(x_j)$$

is called a Gaussian quadrature formula with weight function $w(x)$. We determine the nodes $\{x_i\}$ and weights $\{w_i\}$ by requiring exactness in the above formula for

$$f(x) = x^i, \qquad i = 0, 1, 2, ..., 2n - 1$$

To make the derivation more understandable, we consider the particular case

$$\int_0^1 x^{\frac{1}{3}} f(x)\, dx \approx \sum_{j=1}^{n} w_j f(x_j)$$

We follow the same pattern as used earlier.

The case $n = 1$. We want a formula

$$w_1 f(x_1) \approx \int_0^1 x^{\frac{1}{3}} f(x)\, dx$$

The weight w_1 and the node x_1 are to be so chosen that the formula is exact for polynomials of as large a degree as possible. Choosing $f(x) = 1$, we have

$$w_1 = \int_0^1 x^{\frac{1}{3}}\, dx = \frac{3}{4}$$

Choosing $f(x) = x$, we have

$$\begin{aligned} w_1 x_1 &= \int_0^1 x^{\frac{1}{3}} x\, dx = \frac{3}{7} \\ x_1 &= \frac{4}{7} \end{aligned}$$

Thus

$$\int_0^1 x^{\frac{1}{3}} f(x)\, dx \approx \frac{3}{4} f\left(\frac{4}{7}\right)$$

has degree of precision 1.

The case $n = 2$. We want a formula

$$w_1 f(x_1) + w_2 f(x_2) \approx \int_0^1 x^{\frac{1}{3}} f(x)\,dx$$

The weights w_1, w_2 and the nodes x_1, x_2 are to be so chosen that the formula is exact for polynomials of as large a degree as possible. We determine them by requiring equality for

$$f(x) = 1, x, x^2, x^3$$

This leads to the system

$$\begin{aligned}
w_1 + w_2 &= \int_0^1 x^{\frac{1}{3}}\,dx = \tfrac{3}{4} \\
w_1 x_1 + w_2 x_2 &= \int_0^1 x x^{\frac{1}{3}}\,dx = \tfrac{3}{7} \\
w_1 x_1^2 + w_2 x_2^2 &= \int_0^1 x^2 x^{\frac{1}{3}}\,dx = \tfrac{3}{10} \\
w_1 x_1^3 + w_2 x_2^3 &= \int_0^1 x^3 x^{\frac{1}{3}}\,dx = \tfrac{3}{13}
\end{aligned}$$

The solution is

$$x_1 = \tfrac{7}{13} - \tfrac{3}{65}\,\mathsf{sqrt}(35), \quad x_2 = \tfrac{7}{13} + \tfrac{3}{65}\,\mathsf{sqrt}(35)$$
$$w_1 = \tfrac{3}{8} - \tfrac{3}{392}\,\mathsf{sqrt}(35), \quad w_2 = \tfrac{3}{8} + \tfrac{3}{392}\,\mathsf{sqrt}(35)$$

Numerically,

$$x_1 = .2654117024, \quad x_2 = .8115113746$$
$$w_1 = .3297238792, \quad w_2 = .4202761208$$

The formula

$$\int_0^1 x^{\frac{1}{3}} f(x)\,dx \approx w_1 f(x_1) + w_2 f(x_2) \qquad (4)$$

has degree of precision 3.

EXAMPLE Consider evaluating the integral

$$\int_0^1 x^{\frac{1}{3}} \cos x \, dx \tag{5}$$

In applying (4), we take $f(x) = \cos x$. Then

$$w_1 f(x_1) + w_2 f(x_2) = 0.6074977951$$

The true answer is

$$\int_0^1 x^{\frac{1}{3}} \cos x \, dx \doteq 0.6076257393$$

and our numerical answer is in error by $E_2 \doteq .000128$. This is quite a good answer involving very little computational effort (once the formula has been determined). In contrast, the trapezoidal and Simpson rules applied to (5) would converge very slowly because the first derivative of the integrand is singular at the origin.

CHANGE OF VARIABLES

As a side note to the preceding example, we observe that the change of variables $x = t^3$ transforms the integral (5) to

$$3\int_0^1 t^3 \cos\left(t^3\right)\, dt$$

and both the trapezoidal and Simpson rules will perform better with this formula, although still not as good as our weighted Gaussian quadrature.

A change of the integration variable can often improve the performance of a standard method, usually by increasing the differentiability of the integrand.

EXAMPLE Using $x = t^r$ for some $r > 1$, we have

$$\int_0^1 g(x) \log x\, dx = r\int_0^1 t^{r-1} g\left(t^r\right) \log t\, dt$$

The new integrand is generally smoother than the original one.