Gauss Integration

In the cases considered in the previous two subsections, the function f was mimicked by linear and quadratic functions. These yield exact answers if f itself is a linear or quadratic function (respectively) of x. This process could be continued by increasing the order of the polynomial mimicking-function so as to increase the accuracy with which more complicated functions f could be numerically integrated. However, the same effect can be achieved with less effort by not insisting upon equally spaced points x_i.

The detailed analysis of such methods of numerical integration, in which the integration points are not equally spaced and the weightings given to the values at each point do not fall into a few simple groups, is too long to be given in full here. Suffice it to say that the methods are based upon mimicking the given function with a weighted sum of mutually orthogonal polynomials. The polynomials, $F_n(x)$, are chosen to be orthogonal with respect to a particular weight function $w(x)$, i.e.

$$\int_a^b F_n(x)F_m(x)w(x)\,dx = k_n\delta_{nm},$$

Orthogonal Polynomials obey recurrence relation

$$a_n\varphi_{n+1}(x) = (b_n + c_n x)\varphi_n(x) - d_n\varphi_{n-1}(x)$$

Name	$\varphi_0(x)$	$\varphi_1(x)$	a_n	b_n	c_n	d_n
Legendre	1	x	$n+1$	0	$2n+1$	n
Chebyshev	1	x	1	0	2	1
Laguerre	1	$1-x$	$n+1$	$2n+1$	-1	n
Hermite	1	$2x$	1	0	2	2

Gauss Quadrature

Gauss-Legendre

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell}(x^2-1)^\ell.$$

$$\int_a^b F_n(x) F_m(x) w(x)\, dx = k_n \delta_{nm},$$

interval $-1 \le x \le 1,$

$w(x) = 1$

$$I = \int_a^b f(x)\, dx,$$

$$z = \frac{2x-b-a}{b-a},$$

$$I = \frac{b-a}{2} \int_{-1}^{1} g(z)\, dz,$$

approximate g(x)

$$G(x) = \sum_{i=1}^{n} \frac{P_n(x)}{(x-x_i) P_n'(x_i)}\, g(x_i),$$

i is the ith root of Pi(x)

$$\lim_{x \to x_k} \frac{P_n(x)}{(x-x_i) P_n'(x_i)} = \delta_{ik}.$$

$$\int_{-1}^{1} g(x)\, dx \approx \sum_{i=1}^{n} \frac{g(x_i)}{P_n'(x_i)} \int_{-1}^{1} \frac{P_n(x)}{x-x_i}\, dx.$$

$$w(x_i) \equiv \frac{1}{P_n'(x_i)} \int_{-1}^{1} \frac{P_n(x)}{x-x_i}\, dx \quad = \frac{2}{(1-x_i^2)|P_n'(x_i)|^2}$$

$$\int_{-1}^{1} g(x)\, dx \approx \sum_{i=1}^{n} w_i g(x_i).$$

Exact when g(x) polynomial of order < 2n -1

$$\int_{-1}^{1} f(x)\,dx = \sum_{i=1}^{n} w_i f(x_i)$$

$\pm x_i$	w_i	$\pm x_i$	w_i
$n = 2$		$n = 9$	
0.57735 02692	1.00000 00000	0.00000 00000	0.33023 93550
		0.32425 34234	0.31234 70770
$n = 3$		0.61337 14327	0.26061 06964
0.00000 00000	0.88888 88889	0.83603 11073	0.18064 81607
0.77459 66692	0.55555 55556	0.96816 02395	0.08127 43884
$n = 4$		$n = 10$	
0.33998 10436	0.65214 51549	0.14887 43390	0.29552 42247
0.86113 63116	0.34785 48451	0.43339 53941	0.26926 67193
		0.67940 95683	0.21908 63625
$n = 5$		0.86506 33667	0.14945 13492
0.00000 00000	0.56888 88889	0.97390 65285	0.06667 13443
0.53846 93101	0.47862 86705		
0.90617 98459	0.23692 68851	$n = 12$	
		0.12523 34085	0.24914 70458
$n = 6$		0.36783 14990	0.23349 25365
0.23861 91861	0.46791 39346	0.58731 79543	0.20316 74267
0.66120 93865	0.36076 15730	0.76990 26742	0.16007 83285
0.93246 95142	0.17132 44924	0.90411 72564	0.10693 93260
		0.98156 06342	0.04717 53364
$n = 7$			
0.00000 00000	0.41795 91837	$n = 20$	
0.40584 51514	0.38183 00505	0.07652 65211	0.15275 33871
0.74153 11856	0.27970 53915	0.22778 58511	0.14917 29865
0.94910 79123	0.12948 49662	0.37370 60887	0.14209 61093
		0.51086 70020	0.13168 86384
$n = 8$		0.63605 36807	0.11819 45320
0.18343 46425	0.36268 37834	0.74633 19065	0.10193 01198
0.52553 24099	0.31370 66459	0.83911 69718	0.08327 67416
0.79666 64774	0.22238 10345	0.91223 44283	0.06267 20483
0.96028 98565	0.10122 85363	0.96397 19272	0.04060 14298
		0.99312 85992	0.01761 40071

For our purposes we
only need the table with
w(x) and x.
The weights are
symmetric in + and -

Error is

$$E = \frac{(b-a)^{2n+1}\,(n!)^4}{(2n+1)\left[(2n)!\right]^3} f^{(2n)}(c), \quad a < c < b$$

Gauss-Laguerre

$$\int_0^\infty e^{-x} f(x)\,dx = \sum_{i=1}^{n} w_i f(x_i)$$

$$E = \frac{(n!)^2}{(2n)!} f^{(2n)}(c), \quad 0 < c < \infty$$

x_i	w_i
$n = 2$	
0.58578 64376	0.85355 33906
3.41421 35624	0.14644 66094
$n = 3$	
0.41577 45568	0.71109 30099
2.29428 03603	0.27851 77336
6.28994 50829	0.01038 92565
$n = 4$	
0.32254 76896	0.60315 41043
1.74576 11012	0.35741 86924
4.53662 02969	0.03888 79085
9.39507 09123	0.00053 92947
$n = 5$	
0.26356 03197	0.52175 56106
1.41340 30591	0.39866 68111
3.59642 57710	0.07594 24497
7.08581 00059	0.00361 17587
12.6408 00844	0.00002 33700
$n = 6$	
0.22284 66042	0.45896 46740
1.18893 21017	0.41700 08308
2.99273 63261	0.11337 33821
5.77514 35691	0.01039 91975
9.83746 74184	0.00026 10172
15.9828 73981	0.00000 08985
$n = 7$	
0.19304 36766	0.40931 89517
1.02666 48953	0.42183 12779
2.56787 67450	0.14712 63487
4.90035 30845	0.02063 35145
8.18215 34446	0.00107 40101
12.7341 80292	0.00001 58655
19.3957 27862	0.00000 00317

Gauss-Hermite

$$\int_{-\infty}^\infty e^{-x^2} f(x)\,dx = \sum_{i=1}^{n} w_i f(x_i)$$

$$E = \frac{\sqrt{\pi}\,n!}{2^2(2n)!} f^{(2n)}(c), \quad 0 < c < \infty$$

$\pm x_i$	w_i
$n = 2$	
0.70710 67812	0.88622 69255
$n = 3$	
0.00000 00000	1.18163 59006
1.22474 48714	0.29540 89752
$n = 4$	
0.52464 76233	0.80491 40900
1.65068 01239	0.08131 28354
$n = 5$	
0.00000 00000	0.94530 87205
0.95857 24646	0.39361 93232
2.02018 28705	0.01995 32421
$n = 6$	
0.43607 74119	0.72462 95952
1.33584 90740	0.15706 73203
2.35060 49737	0.00453 00099
$n = 7$	
0.00000 00000	0.81026 46176
0.81628 78829	0.42560 72526
1.67355 16288	0.05451 55828
2.65196 13568	0.00097 17812
$n = 8$	
0.38118 69902	0.66114 70126
1.15719 37124	0.20780 23258
1.98165 67567	0.01707 79830
2.93063 74203	0.00019 96041
$n = 9$	
0.00000 00000	0.72023 52156
0.72355 10188	0.43265 15590
1.46855 32892	0.08847 45274
2.26658 05845	0.00494 36243
3.19099 32018	0.00003 96070

►*Using a 3-point formula in each case, evaluate the integral*

$$I = \int_0^1 \frac{1}{1+x^2}\,dx,$$

(i) *using the trapezium rule,* (ii) *using Simpson's rule,* (iii) *using Gaussian integration. Also evaluate the integral analytically and compare the results.*

(i) Using the trapezium rule, we obtain

$$\begin{aligned} I &= \tfrac{1}{2} \times \tfrac{1}{2}\left[f(0) + 2f\left(\tfrac{1}{2}\right) + f(1)\right] \\ &= \tfrac{1}{4}\left[1 + \tfrac{8}{5} + \tfrac{1}{2}\right] = 0.7750. \end{aligned}$$

(ii) Using Simpson's rule, we obtain

$$\begin{aligned} I &= \tfrac{1}{3} \times \tfrac{1}{2}\left[f(0) + 4f\left(\tfrac{1}{2}\right) + f(1)\right] \\ &= \tfrac{1}{6}\left[1 + \tfrac{16}{5} + \tfrac{1}{2}\right] = 0.7833. \end{aligned}$$

(iii) Using Gaussian integration, we obtain

$$\begin{aligned} I &= \frac{1-0}{2}\int_{-1}^{1} \frac{dz}{1+\frac{1}{4}(z+1)^2} \\ &= \tfrac{1}{2}\left\{0.555\,56\,[f(-0.774\,60) + f(0.774\,60)] + 0.888\,89 f(0)\right\} \\ &= \tfrac{1}{2}\left\{0.555\,56\,[0.987\,458 + 0.559\,503] + 0.888\,89 \times 0.8\right\} \\ &= 0.785\,27. \end{aligned}$$

(iv) Exact evaluation gives

$$I = \int_0^1 \frac{dx}{1+x^2} = \left[\tan^{-1} x\right]_0^1 = \frac{\pi}{4} = 0.785\,40.$$

In practice, a compromise has to be struck between the accuracy of the result achieved and the calculational labour that goes into obtaining it. ◄

Gauss–Chebyshev Quadrature

$$\int_{-1}^{1} \left(1 - x^2\right)^{-1/2} f(x)dx \approx \frac{\pi}{n}\sum_{i=1}^{n} f(x_i) \tag{6.31}$$

Note that all the weights are equal: $A_i = \pi/n$. The abscissas of the nodes, which are symmetric about $x = 0$, are given by

$$x_i = \cos\frac{(2i-1)\pi}{2n} \tag{6.32}$$

The truncation error is

$$E = \frac{2\pi}{2^{2n}(2n)!} f^{(2n)}(c), \quad -1 < c < 1 \tag{6.33}$$

Note the singularity at x = 1

Gauss Quadrature with Logarithmic Singularity

$$\int_0^1 f(x)\ln(x)dx \approx -\sum_{i=1}^{n} A_i f(x_i) \tag{6.38}$$

x_i	A_i	x_i	A_i
$n=2$		$n=5$	
0.112 009	0.718 539	(−1)0.291 345	0.297 893
0.602 277	0.281 461	0.173 977	0.349 776
$n=3$		0.411 703	0.234 488
(−1)0.638 907	0.513 405	0.677314	(−1)0.989 305
0.368 997	0.391 980	0.894 771	(−1)0.189 116
0.766 880	(−1)0.946 154	$n=6$	
$n=4$		(−1)0.216 344	0.238 764
(−1)0.414 485	0.383 464	0.129 583	0.308 287
0.245 275	0.386 875	0.314 020	0.245 317
0.556 165	0.190 435	0.538 657	0.142 009
0.848 982	(−1)0.392 255	0.756 916	(−1)0.554 546
		0.922 669	(−1)0.101 690

Table 6.6. Multiply numbers by 10^k, where k is given in parenthesis

$$E = \frac{k(n)}{(2n)!} f^{(2n)}(c), \quad 0 < c < 1 \tag{6.39}$$

where $k(2) = 0.00\,285$, $k(3) = 0.000\,17$, $k(4) = 0.000\,01$.

EXAMPLE 6.8

Evaluate $\int_{-1}^{1}(1-x^2)^{3/2}dx$ as accurately as possible with Gaussian integration.

Solution As the integrand is smooth and free of singularities, we could use Gauss–Legendre quadrature. However, the exact integral can be obtained with the Gauss–Chebyshev formula. We write

$$\int_{-1}^{1}\left(1-x^2\right)^{3/2}dx = \int_{-1}^{1}\frac{\left(1-x^2\right)^2}{\sqrt{1-x^2}}dx$$

The numerator $f(x) = (1-x^2)^2$ is a polynomial of degree four, so that Gauss–Chebyshev quadrature is exact with three nodes.

The abscissas of the nodes are obtained from Eq. (6.32). Substituting $n = 3$, we get

$$x_i = \cos\frac{(2i-1)\pi}{2(3)}, \quad i = 1, 2, 3$$

Therefore,

$$x_1 = \cos\frac{\pi}{6} = \frac{\sqrt{3}}{2}$$

$$x_2 = \cos\frac{\pi}{2} = 0$$

$$x_2 = \cos\frac{5\pi}{6} = \frac{\sqrt{3}}{2}$$

and Eq. (6.31) yields

$$\int_{-1}^{1}\left(1-x^2\right)^{3/2}dx = \frac{\pi}{3}\sum_{i=1}^{3}\left(1-x_i^2\right)^2$$

$$= \frac{\pi}{3}\left[\left(1-\frac{3}{4}\right)^2 + (1-0)^2 + \left(1-\frac{3}{4}\right)^2\right] = \frac{3\pi}{8}$$

EXAMPLE 6.9

Use Gaussian integration to evaluate $\int_0^{0.5} \cos \pi x \ln x \, dx$.

Solution We split the integral into two parts:

$$\int_0^{0.5} \cos \pi x \ln x \, dx = \int_0^1 \cos \pi x \ln x \, dx - \int_{0.5}^1 \cos \pi x \ln x \, dx$$

The first integral on the right-hand side, which contains a logarithmic singularity at $x = 0$, can be computed with the special Gaussian quadrature in Eq. (6.38). Choosing $n = 4$, we have

$$\int_0^1 \cos \pi x \ln x \, dx \approx -\sum_{i=1}^{4} A_i \cos \pi x_i$$

where x_i and A_i are given in Table 6.7. The sum is evaluated in the following table:

x_i	$\cos \pi x_i$	A_i	$A_i \cos \pi x_i$
0.041 448	0.991 534	0.383 464	0.380 218
0.245 275	0.717 525	0.386 875	0.277 592
0.556 165	−0.175 533	0.190 435	−0.033 428
0.848 982	−0.889 550	0.039 225	−0.034 892
			$\Sigma = 0.589\,490$

Thus

$$\int_0^1 \cos \pi x \ln x \, dx \approx -0.589\,490$$

The second integral is free of singularities, so that it can be evaluated with Gauss–Legendre quadrature. Choosing again $n = 4$, we have

$$\int_{0.5}^{1} \cos \pi x \ln x \, dx \approx 0.25 \sum_{i=1}^{4} A_i \cos \pi x_i \ln x_i$$

where the nodal abscissas are – see Eq. (6.28)

$$x_i = \frac{1 + 0.5}{2} + \frac{1 - 0.5}{2} \xi_i = 0.75 + 0.25 \xi_i$$

Looking up ξ_i and A_i in Table 6.3 leads to the following computations:

ξ_i	x_i	$\cos \pi x_i \ln x_i$	A_i	$A_i \cos \pi x_i \ln x_i$
−0.861 136	0.534 716	0.068 141	0.347 855	0.023 703
−0.339 981	0.665 005	0.202 133	0.652 145	0.131 820
0.339 981	0.834 995	0.156 638	0.652 145	0.102 151
0.861 136	0.965 284	0.035 123	0.347 855	0.012 218
				$\Sigma = 0.269\,892$

from which

$$\int_{0.5}^{1} \cos \pi x \ln x \, dx \approx 0.25(0.269\,892) = 0.067\,473$$

Therefore,

$$\int_{0}^{1} \cos \pi x \ln x \, dx \approx -0.589\,490 - 0.067\,473 = -0.656\,96\,3$$

which is correct to six decimal places.

EXAMPLE 6.10

Evaluate as accurately as possible

$$F = \int_0^\infty \frac{x+3}{\sqrt{x}} e^{-x} dx$$

EXAMPLE 6.10

Evaluate as accurately as possible

$$F = \int_0^\infty \frac{x+3}{\sqrt{x}} e^{-x} dx$$

Solution In its present form, the integral is not suited to any of the Gaussian quadratures listed in this section. But using the transformation

$$x = t^2 \qquad dx = 2t\,dt$$

the integral becomes

$$F = 2\int_0^\infty (t^2+3)e^{-t^2}\,dt = \int_{-\infty}^\infty (t^2+3)e^{-t^2}\,dt$$

which can be evaluated exactly with Gauss–Hermite formula using only two nodes ($n = 2$). Thus

$$\begin{aligned} F &= A_1(t_1^2+3) + A_2(t_2^2+3) \\ &= 0.886\,227\left[(0.707\,107)^2+3\right] + 0.886\,227\left[(-0.707\,107)^2+3\right] \\ &= 6.203\,59 \end{aligned}$$

EXAMPLE 6.11

Determine how many nodes are required to evaluate

$$\int_0^{\pi} \left(\frac{\sin x}{x}\right)^2 dx$$

with Gauss–Legendre quadrature to six decimal places. The exact integral, rounded to six places, is 1.418 15.

Solution The integrand is a smooth function; hence, it is suited for Gauss–Legendre integration. There is an indeterminacy at $x = 0$, but this does not bother the quadrature since the integrand is never evaluated at that point. We used the following program that computes the quadrature with 2, 3, . . . , nodes until the desired accuracy is reached:

```
% Example 6.11 (Gauss-Legendre quadrature)
func = @(x) ((sin(x)/x)^2);
a = 0; b = pi; Iexact = 1.41815;
for n = 2:12
    I = gaussQuad(func,a,b,n);
    if abs(I - Iexact) < 0.00001
        I
        n
        break
    end
end
```

The program produced the following output:

```
I =
   1.41815026780139
n =
     5
```

EXAMPLE 6.12

Evaluate numerically $\int_{1.5}^{3} f(x)\,dx$, where $f(x)$ is represented by the unevenly spaced data

x	1.2	1.7	2.0	2.4	2.9	3.3
$f(x)$	−0.362 36	0.128 84	0.416 15	0.737 39	0.970 96	0.987 48

Knowing that the data points lie on the curve $f(x) = -\cos x$, evaluate the accuracy of the solution.

Since the polynomial is of degree five, only three nodes ($n = 3$) are required in the quadrature.

From Eq. (6.28) and Table 6.6, we obtain the abscissas of the nodes

$$x_1 = \frac{3+1.5}{2} + \frac{3-1.5}{2}(-0.774597) = 1.6691$$

$$x_2 = \frac{3+1.5}{2} = 2.25$$

$$x_3 = \frac{3+1.5}{2} + \frac{3-1.5}{2}(0.774597) = 2.8309$$

We now compute the values of the interpolant $P_5(x)$ at the nodes. This can be done using the functions `newtonPoly` or `neville` listed in Section 3.2. The results are

$$P_5(x_1) = 0.098\,08 \qquad P_5(x_2) = 0.628\,16 \qquad P_5(x_3) = 0.952\,16$$

Using Gauss–Legendre quadrature

$$I = \int_{1.5}^{3} P_5(x)dx = \frac{3-1.5}{2}\sum_{i=1}^{3} A_i P_5(x_i)$$

we get

$$\begin{aligned} I &= 0.75\,[0.555\,556(0.098\,08) + 0.888\,889(0.628\,16) + 0.555\,556(0.952\,16)] \\ &= 0.856\,37 \end{aligned}$$