Numerical Integration

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Newton - Cotes integration formulas

The Newton-Cotes technique for numerical integrations is similar to the one for finding numerical derivatives of functions. That is, we create the interpolating polynomial of degree $P_n(x)$ for a given function $y(x)$. Then instead of integrating the function we integrate the polynomial i.e.

$$\int_a^b y(x)dx \to \int_a^b P_n(x)dx \tag{1}$$

where ($x_s = x_0 + sh$)

$$P_n(x_s) = f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 f_0 + ... \tag{2}$$

The formulas that one can derive depend on the number of terms of the interpolating polynomial that we will use. The error will be estimate from the integration of the error of the interpolating polynomial used, i.e.

$$E = \int_a^b E_n(x_s)dx \tag{3}$$

where

$$E_n(x_s) = \frac{s(s-1)(s-2)...(s-n)}{(n+1)!}h^{n+1}f^{(n+1)}(\xi) \quad \text{where} \quad \xi \in [a, b] \tag{4}$$

1st order interpolating polynomial

If we use a 1st order interpolating polynomial we get:

$$\int_{x_0}^{x_1} f(x)dx \quad \rightarrow \quad \int_{x_0}^{x_1} P_1(x_s)dx = \int_{x_0}^{x_1} (f_0 + s\Delta f_0)\, dx = h\int_{s=0}^{s=1} (f_0 + s\Delta f_0)\, ds$$

$$= \quad [hf_0 s]_0^1 + \left[h\Delta f_0 \frac{s^2}{2}\right]_0^1 = h\left(f_0 + \frac{1}{2}\Delta f_0\right) = \frac{h}{2}(f_0 + f_1) \qquad (5)$$

The error introduced when a 1st order polynomial is used is:

$$f(x) - P(x) = \frac{1}{2}s(s-1)h^2 f''(\xi) \quad \text{for} \quad x_0 \leq \xi \leq x_1 \qquad (6)$$

Then the error in the relation for numerical integration will be estimated by integrating the above relation

$$E \quad = \quad \int_{x_0}^{x_1} \frac{1}{2}s(s-1)h^2 f''(\xi)dx = \frac{h^3}{2}\int_{s=0}^{s=1} s(s-1)f''(\xi)ds$$

$$= \quad h^3 f''(\xi_1)\left(\frac{s^3}{6} - \frac{s^2}{4}\right)_0^1 = -\frac{1}{12}h^3 f''(\xi_1) \quad \text{where} \quad \xi_1 \in [x_0, x_1] \quad (7)$$

2nd order interpolating polynomial

Following the previous procedure we get

$$\begin{aligned}
\int_{x_0}^{x_2} f(x)dx \quad \rightarrow \quad \int_{x_0}^{x_2} P_2(x_s)dx &= \int_{x_0}^{x_2} \left(f_0 + s\Delta f_0 + \frac{1}{2}s(s-1)\Delta^2 f_0\right) dx \\
&= h\int_{s=0}^{s=2} \left(f_0 + s\Delta f_0 + \frac{1}{2}s(s-1)\Delta^2 f_0\right) ds \\
&= h\left(2f_0 + 2\Delta f_0 + \frac{1}{3}\Delta^2 f_0\right) = \frac{h}{3}\left(f_0 + 4f_1 + f_2\right) \qquad (8)
\end{aligned}$$

It happens that the integration of the corresponding error term in our this case gives zero, i.e.

$$\frac{h^3}{3!}\int_0^2 s(s-1)(s-2)f^{(3)}(\xi)ds = 0\,. \qquad (9)$$

Which means that due to this coincidence the error will be smaller than what one my expect and will be estimated by integrating the next term

$$E = \frac{h^4}{4!}\int_0^2 s(s-1)(s-2)(s-3)f^{(4)}(\xi)ds = \ldots = -\frac{1}{90}h^5 f^{(4)}(\xi_1) \qquad (10)$$

where $\xi_1 \in [x_0, x_2]$.

3rd order interpolating polynomial

Following the previous procedure we get

$$\int_{x_0}^{x_3} f(x)dx \to \int_{x_0}^{x_3} P_3(x_s)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)\,. \tag{11}$$

In a similar way we get the error:

$$E = -\frac{3}{80}h^5 f^{(4)}(\xi_1) \quad \text{for} \quad \xi_1 \in [x_0, x_3] \tag{12}$$

I.e. the error is $O(h^5)$ which is of the same order as the error found earlier by using an interpolating polynomial of 2nd order.

This "coincidence" in the order of the errors happens also for 4th and 5th order interpolating polynomials which give an error of the order of $O(h^7)$.

Newton – Cotes Formulae

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{1}{12}h^3 f^{(2)}(\xi_1)$$

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{1}{90}h^5 f^{(4)}(\xi_1)$$

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3}{80}h^5 f^{(4)}(\xi_1)$$

Table 1: Newton-Cotes for numerical integration by using 1st, 2nd and 3rd order interpolating polynomials

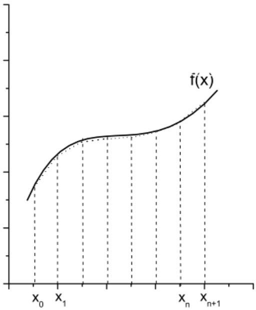
The trapezoidal rule

If the interval (a, b) is quite long then we subdivide it into n subintervals i.e.$\{a = x_0, ..., x_n = b; n\}$ with $h = \Delta x = x_{i+1} - x_i = (b-a)/n$

$$\begin{aligned}
\int_a^b f(x)dx &= \int_{x_0}^{x_n} f(x)dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} P_1(x)dx \\
&= \int_{x_0}^{x_1} P_1(x)dx + \int_{x_1}^{x_2} P_1(x)dx + ... + \int_{x_{n-1}}^{x_n} P_1(x)dx \\
&= \sum_{i=0}^{n-1} \frac{h}{2}(f_i + f_{i+1}) = \frac{h}{2}(f_0 + 2f_1 + ... + 2f_{n-1} + f_n) \qquad (13)
\end{aligned}$$

Global Error:

$$\begin{aligned}
E &= -\frac{h^3}{12}\left[f''(\xi_1) + f''(\xi_2) + ... + f''(\xi_n)\right] \approx -\frac{h^3}{12} n f''(\xi) \\
&= -\frac{h^2}{12}(b-a)f''(\xi) \quad \text{where} \quad a \le \xi \le b \qquad (14)
\end{aligned}$$


f(x)
x0
x1
xn
xn+1

Simpson's rules

Simpson's 1/3 rule

$$\int_{a=x_0}^{b=x_n} f(x)dx = \sum_{i=0}^{n-2} \int_{x_i}^{x_{i+2}} P_2(x)dx = \sum_{i=0}^{n-2} \frac{h}{3}\left(f_i + 4f_{i+1} + f_{i+2}\right)$$
$$= \frac{h}{3}\left(f_1 + 4f_2 + 2f_3 + 4f_4 + \ldots + 2f_{n-2} + 4f_{n-1} + f_n\right) \quad (15)$$

Global Error:

$$E = -\frac{h^5}{90}\frac{n}{2}f^{(4)}(\xi) = -\frac{b-a}{180}h^4 f^{(4)}(\xi) \quad \text{for} \quad a \leq \xi \leq b \quad (16)$$

Simpson's 3/8 rule

$$\int_{a=x_0}^{b=x_n} f(x)\,dx = \frac{3h}{8}\left(f_0 + 3f_1 + 3f_2 + 2f_3 + \ldots + 2f_{n-3} + 3f_{n-2} + 3f_{n-1} + f_n\right) \quad (17)$$

Global Error:

$$E = -\frac{b-a}{80}h^4 f^{(4)}(\xi) \quad \text{for} \quad a \leq \xi \leq b \quad (18)$$

Formulas for integration

$$\begin{aligned}
\int_{x_0}^{x_n} f(x)dx &= \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + ... + 2f_{n-1} + f_n\right) \\
&- \frac{b-a}{12} h^2 f^{(2)}(\xi_1) \\
\int_{x_0}^{x_n} f(x)dx &= \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + ... + 2f_{n-2} + 4f_n + f_{n+1}\right) \\
&- \frac{b-a}{180} h^4 f^{(4)}(\xi_1) \quad \text{requires an even number of panels} \\
\int_{x_0}^{x_n} f(x)dx &= \frac{3h}{8}\left(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + ... + 3f_{n-2} + 3f_{n-1} + f_n\right) \\
&- \frac{b-a}{80} h^4 f^{(4)}(\xi_1) \quad \text{number of panels divisible by 3} \\
&\text{where} \quad x_0 \leq \xi_1 \leq x_n
\end{aligned}$$

Romberg integration i

- for step h: True value $A = I_1 + ch^2$
- for step kh: True value $A = I_2 + c\,(kh)^2$

from which we get:

$$A = \frac{k^2 I_1 - I_2}{k^2 - 1} \quad \text{and} \quad c = \frac{I_2 - I_1}{h^2(1 - k^2)} \tag{19}$$

which for example for $k = 1/2$ gives

$$A = I_2 + \frac{1}{3}\,(I_2 - I_1) \tag{20}$$

and in the general case for methods with error $O(h^n)$ and $k = 1/2$ we can get:

$$A = I_2 + \frac{I_2 - I_1}{2^n - 1}\,. \tag{21}$$

Application

If we start with the trapezoidal rule

$$
\begin{aligned}
I_1 &= \frac{2h}{2}(f_0 + f_2) = h(f_0 + f_2) \\
I_2 &= \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) = \frac{h}{2}(f_0 + 2f_1 + f_2)
\end{aligned}
$$

then the **true value**, according to (20), will be

$$
A = \frac{2h(f_0 + 2f_1 + f_2) - h(f_0 + f_2)}{3} = \frac{h}{3}(f_0 + 4f_1 + f_2) \quad !!!
$$

EXERCISE: Test numerically the Romberg method for the Simpson 1/3 formula.

Splines and integration

For every interval $[x_i, x_{i+1}]$ we will have a 3rd order polynomial i.e.

$$\begin{aligned}
\int_{x_0}^{x_n} f(x)dx &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx \\
&= \sum_{i=0}^{n-1} \left[\frac{a_i}{4}(x - x_i)^4 + \frac{b_i}{3}(x - x_i)^3 + \frac{c_i}{2}(x - x_i)^2 + d_i(x - x_i) \right]_{x_i}^{x_{i+1}} \\
&= \sum_{i=0}^{n-1} \left[\frac{a_i}{4}(x_{i+1} - x_i)^4 + \frac{b_i}{3}(x_{i+1} - x_i)^3 + \frac{c_i}{2}(x_{i+1} - x_i)^2 + d_i(x_{i+1} - x_i) \right] .
\end{aligned}$$

$$\int_{x_0}^{x_n} f(x)dx = \frac{h^4}{4} \sum_{i=0}^{n-1} a_i + \frac{h^3}{3} \sum_{i=0}^{n-1} b_i + \frac{h^2}{2} \sum_{i=0}^{n-1} c_i + h \sum_{i=0}^{n-1} d_i \qquad (22)$$

Mean value theorem:

$$\int_a^b f(x)\,dx = (b-a)\,f(\xi) \tag{23}$$

We can get an approximate value for the integral by writting

$$I = \int_a^b f(x)dx \equiv c_0 f(a) + c_1 f(b) \tag{24}$$

This will be exact for polynomials of the form $f(x) = 1$ and $f(x) = x$

$$f(x) = x \quad \Rightarrow \quad \int_a^b x \cdot dx = \left.\frac{x^2}{2}\right|_a^b = \frac{1}{2}\left(b^2 - a^2\right) \equiv c_0 \cdot a + c_1 \cdot b \tag{25}$$

$$f(x) = 1 \quad \Rightarrow \quad \int_a^b 1 \cdot dx = x|_a^b = (b-a) \equiv c_0 \cdot 1 + c_1 \cdot 1 \tag{26}$$

$$c_0 = \frac{b-a}{2} \quad \text{and} \quad c_1 = \frac{b-a}{2} \tag{27}$$

Thus

$$\int_a^b f(x)dx \equiv \frac{b-a}{2}\left[f(a) + f(b)\right] \tag{28}$$

If we continue by creating according to (24), an relation with 3 terms we get:

$$\int_a^b f(x)dx \equiv c_0 f(a) + c_1 f\left(\frac{a+b}{2}\right) + c_2 f(b) \tag{29}$$

This will be exact for polynomials of the form $f(x) = 1$, $f(x) = x$ and $f(x) = x^2$ and we can get:

$$\int_a^b f(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \tag{30}$$

Euler-Maclaurin Formula i

This procedure can be extended by using the derivatives i.e.

$$\int_a^b f(x)dx = c_0 f(a) + c_1 f(b) + c_2 f'(a) + c_3 f'(b) \tag{31}$$

which can be generalized to the Euler-Maclaurin formula

$$\begin{aligned}\int_{x_0}^{x_n} f(x)\,dx &= \frac{h}{2}\left[f(x_0) + 2f(x_1) + \ldots + 2f(x_{n-1}) + f(x_n)\right] \\ &- \frac{h^2}{12}\left[f'(x_n) - f'(x_0)\right] \\ &+ \frac{h^4}{720}\left[f^{(3)}(x_n) - f^{(3)}(x_0)\right] \\ &- \frac{h^6}{30240}\left[f^{(5)}(x_n) - f^{(5)}(x_0)\right]\end{aligned} \tag{32}$$

Example

$$I = \int_0^{\pi/2} \sin(x)dx$$

By using the formula (32) for only 2 points at the ends of the interval we get:

$$\begin{aligned}
\int_0^{\pi/2} \sin(x)dx &= \frac{\pi}{4}\left(\sin 0 + \sin\frac{\pi}{2}\right) \quad (= 0.785398) \\
&+ \frac{\pi^2}{2^2 \cdot 12}\left(\cos 0 - \cos\frac{\pi}{2}\right) \quad (= 0.991015) \\
&- \frac{\pi^4}{2^4 \cdot 720}\left(\sin 0 - \sin\frac{\pi}{2}\right) \quad (= 0.999471) \\
&+ \frac{\pi^6}{2^6 \cdot 30240}\left(\cos 0 - \cos\frac{\pi}{2}\right) \quad (= 0.999967) \\
&= \frac{\pi}{4} + \frac{\pi^2}{48} + \frac{\pi^4}{16 \cdot 720} + \frac{\pi^6}{2^6 \cdot 30240} = 0.99996732 \\
&\quad \text{Error} \sim 3 \times 10^{-5}.
\end{aligned}$$

Filon's method i

For integral of the type

$$\int_a^b f(x)\sin(x)dx \quad \text{and} \quad \int_a^b f(x)\cos(x)dx$$

we can try

$$\int_0^{2\pi} f(x)\sin(x)dx \approx A_1 f(0) + A_2 f(\pi) + A_3 f(2\pi)$$

which will be true for $f(x) = 1$, $f(x) = x$ and $f(x) = x^2$

$$\begin{aligned} f(x) = 1 \qquad &\Rightarrow \quad 0 = A_1 + A_2 + A_3 \\ f(x) = x \qquad &\Rightarrow \quad -2\pi = \pi A_2 + 2\pi A_3 \\ f(x) = x^2 \qquad &\Rightarrow \quad -4\pi^2 = \pi^2 A_2 + 4\pi^2 A_3 \end{aligned}$$

with solution $A_1 = 1$, $A_2 = 0$ and $A_3 = -1$.Thus

$$\int_0^{2\pi} f(x)\sin x dx \approx f(0) - f(2\pi)\,.$$

For $f(x) = x^3$ the exact value is ≈ -210 and the approximate one ≈ -248.

Filon's method ii

the General Formula

$$\int_a^b y(x)\sin(kx)dx \approx h\left[Ay(a)\cos(ka) - Ay(b)\cos(kb) + BS_e + DS_o\right] \quad (33)$$

$$\int_a^b y(x)\cos(kx)dx \approx h\left[Ay(a)\cos(ka) - Ay(b)\cos(kb) + BC_e + DC_o\right] \quad (34)$$

$$A = \frac{1}{q} + \frac{\sin(2q)}{2q^2} - \frac{2\sin^2(q)}{q^3} \quad (35)$$

$$B = \frac{1}{q^2} + \frac{\cos^2(q)}{q^2} - \frac{\sin(2q)}{q^3} \quad (36)$$

$$D = \frac{4\sin(q)}{q^3} - \frac{4\cos(q)}{q^2} \quad (37)$$

Filon's method iii

$$S_e = -y(a)\sin(ka) - y(b)\sin(kb) + 2\sum_{i=0}^{n} y(a+2ih)\sin(ka+2iq) \quad (38)$$

$$S_o = \sum_{i=1}^{n} y\left[a+(2i-1)h\right]\sin\left[ka+(2i-1)q\right] \quad (39)$$

$$C_e = -y(a)\sin(ka) - y(b)\sin(kb) + 2\sum_{i=0}^{n} y(a+2ih)\sin(ka+2iq) \quad (40)$$

$$C_o = \sum_{i=1}^{n} y\left[a+(2i-1)h\right]\sin\left[ka+(2i-1)q\right] \quad (41)$$

where $q = kh$.

Example

$$I = \int_0^{2\pi} e^{-x/2} \cos(100x) dx = \frac{2\left(1 - e^{-\pi}\right)}{40001} \approx 4.783810813 \times 10^{-5} \qquad (42)$$

Notice that Filon's method with only 4 points outperforms Simpson's method with 1000 points

n	Simpson	Filon
4	1.91733833E+0	4.77229440E-5
8	-5.73192992E-2	4.72338540E-5
16	2.42801799E-2	4.72338540E-5
128	5.55127202E-4	4.78308678E-5
256	-1.30263888E-4	4.78404787E-5
1024	4.77161559E-5	4.78381120E-5
2048	4.78309107E-5	4.78381084E-5

It is an extension of the previous techniques but instead of fixing the points of the interval we calculate them together with the weighting coefficients. For example

$$\int_{-1}^{1} f(x)dx \approx af(x_1) + bf(x_2) \tag{43}$$

this integral can be exact for $f(x) = 1$, $f(x) = x$, $f(x) = x^2$ and $f(x) = x^3$. Thus we get the following system of equations:

$$\left.\begin{array}{lll} f(x) = 1 & \Rightarrow & 2 = a + b \\ f(x) = x & \Rightarrow & 0 = ax_1 + bx_2 \\ f(x) = x^2 & \Rightarrow & \frac{2}{3} = ax_1^2 + bx_2^2 \\ f(x) = x^3 & \Rightarrow & 0 = ax_1^3 + bx_2^3 \end{array}\right\} \Rightarrow \quad \begin{array}{l} a = b = 1 \\ x_1 = -x_2 = -\left(\frac{1}{3}\right)^{1/2} = -0.5773 \end{array}$$

$$\int_{-1}^{1} f(x)dx \approx f(-0.5773) + f(0.5773)$$

Thus we need to evaluate the function only at only 2 appropriate points which are: $x_1 = -0.5773$ and $x_2 = 0.5773$.

For arbitrary end-points we use the transformation:

$$t = \frac{1}{2}(b-a)x + \frac{1}{2}(b+a) \quad \text{and} \quad dt = \frac{b-a}{2}dx\,. \tag{44}$$

EXAMPLE

$$I = \int_0^{\pi/2} \sin(x)dx$$

We change the variable of integration to get the limits of integration -1 and 1

$$x = \frac{1}{2}\left(\frac{\pi}{2}t + \frac{\pi}{2}\right) = \frac{\pi}{4}(t+1) \quad \text{and} \quad dx = \frac{\pi}{4}dt$$

and the new integral is:

$$\begin{aligned} I &= \frac{\pi}{4}\int_{-1}^{1} \sin\left[\frac{\pi}{4}(t+1)\right] dt \\ &= \frac{\pi}{4}\left[1.0 \times \sin(0.10566 \times \pi) + 1.0 \times \sin(0.39434 \times \pi)\right] = 0.99849 \end{aligned}$$

i.e. an error 1.53×10^{-3} while the 2 point trapezoidal rule gives $I = 0.7854$ and Simposn's 3 point formula 1.0023.

Gauss-Legendre method

It is a generalization of Gauss' method of n points, i.e. if

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} A_i f(x_i) \tag{45}$$

we have to solve a system of $2n$ equations to calculate the $2n$ quantities A and x_i. This method will be exact for polynomials up to degree $2(n-1)$ thus the $2n$ equations can be written as:

$$A_1 x_1^k + ... + A_n x_n^k = \begin{cases} 0 \quad \text{for} \quad k = 1, 3, 5, ..., 2n-1 \\ \\ \frac{2}{k+1} \quad \text{for} \quad k = 2, 4, 6, ..., 2n-2 \end{cases} \tag{46}$$

It can be proved that the x_i are roots of the Legendre polynomial of nth-degree which can be always found in the interval $(-1, 1)$.
The Legendre polynomials can be derived from the recursion relation:

$$(n+1) L_{n+1}(x) - (2n+1) x L_n(x) + n L_{n-1}(x) = 0 \tag{47}$$

where the first 3 are:

$$L_0(x) = 1, \qquad L_1(x) = x \quad \text{and} \quad L_2(x) = \frac{3}{2}x^2 - \frac{1}{2} \tag{48}$$

Then the A_i are estimated from:

$$A_i = \frac{2\left(1 - x^2\right)}{n^2\left[L_{n-1}\left(x_i\right)\right]^2} \tag{49}$$

For example, if $n = 4$ we should find the roots of 4th-degree Legendre polynomial

$$P_4 = \frac{1}{8}\left(35x^4 - 30x^2 + 3\right)$$

which are $x_i = \pm\left[(15 \pm 2\sqrt{30})/35\right]^{1/2}$ and then by using (49) to calculate A_i. The exact values are given in the Table 2

n	x_i	A_i
2	$\pm$ 0.5773502692	1.000000000
4	$\pm$ **0.8611363116**	0.3478548451
	$\pm$ **0.3394810436**	0.6521451549
8	$\pm$ 0.9602898565	0.1012285363
	$\pm$ 0.7966664774	0.2223810345
	$\pm$ 0.5255324099	0.3137066459
	$\pm$ 0.1834346425	0.3626837834

Table 2: The values of x_i and A_i for the Gauss-Legendre for 2, 4 and 8 points.

Table 25.4 ABSCISSAS AND WEIGHT FACTORS FOR GAUSSIAN INTEGRATION

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

Abscissas $=\pm x_i$ (Zeros of Legendre Polynomials) Weight Factors $=w_i$

n	$\pm x_i$	w_i
$n=2$	0.57735 02691 89626	1.00000 00000 00000
$n=3$	0.00000 00000 00000	0.88888 88888 88889
	0.77459 66692 41483	0.55555 55555 55556
$n=4$	0.33998 10435 84856	0.65214 51548 62546
	0.86113 63115 94053	0.34785 48451 37454
$n=5$	0.00000 00000 00000	0.56888 88888 88889
	0.53846 93101 05683	0.47862 86704 99366
	0.90617 98459 38664	0.23692 68850 56189
$n=6$	0.23861 91860 83197	0.46791 39345 72691
	0.66120 93864 66265	0.36076 15730 48139
	0.93246 95142 03152	0.17132 44923 79170
$n=7$	0.00000 00000 00000	0.41795 91836 73469
	0.40584 51513 77397	0.38183 00505 05119
	0.74153 11855 99394	0.27970 53914 89277
	0.94910 79123 42759	0.12948 49661 68870
$n=8$	0.18343 46424 95650	0.36268 37833 78362
	0.52553 24099 16329	0.31370 66458 77887
	0.79666 64774 13627	0.22238 10344 53374
	0.96028 98564 97536	0.10122 85362 90376
$n=9$	0.00000 00000 00000	0.33023 93550 01260
	0.32425 34234 03809	0.31234 70770 40003
	0.61337 14327 00590	0.26061 06964 02935
	0.83603 11073 26636	0.18064 81606 94857
	0.96816 02395 07626	0.08127 43883 61574
$n=10$	0.14887 43389 81631	0.29552 42247 14753
	0.43339 53941 29247	0.26926 67193 09996
	0.67940 95682 99024	0.21908 63625 15982
	0.86506 33666 88985	0.14945 13491 50581
	0.97390 65285 17172	0.06667 13443 08688
$n=12$	0.12523 34085 11469	0.24914 70458 13403
	0.36783 14989 98180	0.23349 25365 38355
	0.58731 79542 86617	0.20316 74267 23066
	0.76990 26741 94305	0.16007 83285 43346
	0.90411 72563 70475	0.10693 93259 95318
	0.98156 06342 46719	0.04717 53363 86512
$n=16$	0.09501 25098 37637 440185	0.18945 06104 55068 496285
	0.28160 35507 79258 913230	0.18260 34150 44923 588867
	0.45801 67776 57227 386342	0.16915 65193 95002 538189
	0.61787 62444 02643 748447	0.14959 59888 16576 732081
	0.75540 44083 55003 033895	0.12462 89712 55533 872052
	0.86563 12023 87831 743880	0.09515 85116 82492 784810
	0.94457 50230 73232 576078	0.06225 35239 38647 892863
	0.98940 09349 91649 932596	0.02715 24594 11754 094852
$n=20$	0.07652 65211 33497 333755	0.15275 33871 30725 850698
	0.22778 58511 41645 078080	0.14917 29864 72603 746788
	0.37370 60887 15419 560673	0.14209 61093 18382 051329
	0.51086 70019 50827 098004	0.13168 86384 49176 626898
	0.63605 36807 26515 025453	0.11819 45319 61518 417312
	0.74633 19064 60150 792614	0.10193 01198 17240 435037
	0.83911 69718 22218 823395	0.08327 67415 76704 748725
	0.91223 44282 51325 905868	0.06267 20483 34109 063570
	0.96397 19272 77913 791268	0.04060 14298 00386 941331
	0.99312 85991 85094 924786	0.01761 40071 39152 118312
$n=24$	0.06405 68928 62605 626085	0.12793 81953 46752 156974
	0.19111 88674 73616 309159	0.12583 74563 46828 296121
	0.31504 26796 96163 374387	0.12167 04729 27803 391204
	0.43379 35076 26045 138487	0.11550 56680 53725 601353
	0.54542 14713 88839 535658	0.10744 42701 15965 634783
	0.64809 36519 36975 569252	0.09761 86521 04113 888270
	0.74012 41915 78554 364244	0.08619 01615 31953 275917
	0.82000 19859 73902 921954	0.07334 64814 11080 305734
	0.88641 55270 04401 034213	0.05929 85849 15436 780746
	0.93827 45520 02732 758524	0.04427 74388 17419 806169
	0.97472 85559 71309 498198	0.02853 13886 28933 663181
	0.99518 72199 97021 360180	0.01234 12297 99987 199547

Compiled from P. Davis and P. Rabinowitz, Abscissas and weights for Gaussian quadratures of high order, J. Research NBS **56**, 35–37, 1956, RP2645; P. Davis and P. Rabinowitz, Additional abscissas and weights for Gaussian quadratures of high order. Values for $n=64$, 80, and 96, J. Research NBS **60**, 613–614, 1958, RP2875; and A. N. Lowan, N. Davids, and A. Levenson, Table of the zeros of the Legendre polynomials of order 1–16 and the weight coefficients for Gauss' mechanical quadrature formula, Bull. Amer. Math. Soc. 48, 739–743, 1942 (with permission).

Generalization of Gauss's method

For integrals of the type

$$I = \int_a^b w(x)y(x)dx \tag{50}$$

one can uses alternative orthogonal polynomials, and by writing

$$\int_a^b w(x)y(x)dx = \sum_{i=1}^{n} A_i y(x_i) \tag{51}$$

the unknowns x_i and A_i can be found from tables in mathematical handbooks. Depending on the form of the weighting function $w(x)$ we have the following choices:

- **Gauss-Legendre method** for weighting function $w(x) = 1$.
- **Gauss-Laguerre method** for integrals of the form

$$\int_0^\infty e^{-x} y\left(x\right) dx \approx \sum_{i=1}^{n} A_i y\left(x_i\right) \tag{52}$$

with weighting function $w(x) = e^{-x}$ where x_i are roots of the Laguerre polynomials which can be created from the recursion:

$$L_n(x) = e^x \frac{d^n}{dx^n}\left(e^{-x}x^n\right) \tag{53}$$

while the coefficients A_i will be given by:

$$A_i = \frac{(n!)^2}{x_i\left[L_n'(x_i)\right]^2} \tag{54}$$

n	x_i	A_i
2	0.58578644	0.85355339
	3.41421356	0.14644661
4	0.32254769	0.60315410
	1.74576110	0.35741869
	4.53662030	0.03888791
	9.39507091	0.00053929
6	0.22284660	0.10122854
	1.18893210	0.41700083
	2.99273633	0.11337338
	5.77514357	0.01039920
	9.83746742	0.00026102
	15.98287398	0.00000090

Table 3: The values of x_i and A_i of Gauss-Laguerre method for 2, 4 and 6 points.

- **Gauss-Hermite method** for integrals of the form

$$\int_{-\infty}^{\infty} e^{-x^2} y(x) dx \approx \sum_{i=1}^{n} A_i y(x_i) \tag{55}$$

i.e. the weighting function is $w(x) = e^{-x^2}$ while the x_i are roots of the Hermite polynomials. The Hermite polynomials can be created via the relation

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left(e^{-x^2} \right) \tag{56}$$

while the coefficients A_i can be found by the relation:

$$A_i = \frac{2^{n+1} n! \sqrt{\pi}}{[H_n'(x_i)]^2} \tag{57}$$

Both x_i and A_i are given in Table 4.

n	x_i	A_i
2	$\pm$ 0.70710678	0.88622693
4	$\pm$ 0.52464762	0.80491409
	$\pm$ 1.65068012	0.08131284
6	$\pm$ 0.43607741	0.72462960
	$\pm$ 1.33584907	0.15706732
	$\pm$ 2.35060497	0.00453001

Table 4: The values x_i and A_i of the Gauss-Hermite method for 2, 4 and 6 points.

- **Gauss-Chebyshev method** for integrals of the form:

$$\int_{-1}^{1} \frac{y(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{n} \sum_{i=1}^{n} y(x_i) \tag{58}$$

i.e. the weighting function is

$$w(x) = \frac{1}{\sqrt{1-x^2}} \tag{59}$$

while the x_i are the roots of the Chebyshev polynomials

$$T_n(x) = \cos\left[n \arccos(x)\right] \tag{60}$$

and given by the relations

$$x_i = \cos\left[\frac{\pi}{2n}(2i-1)\right] . \tag{61}$$

While the A_i are given by

$$A_i = \frac{\pi}{n} \tag{62}$$

where n is the degree of the polynomial that we use.

Improper and Indefinite integrals

For example:

$$I = \int_0^\infty xe^{-x} dx$$

this can be written as

$$I = \int_0^1 xe^{-x} dx + \int_1^\infty xe^{-x} dx$$

and substitute $y = 1/x$ in the 2nd part

But in general we can write it in the form

$$I = \lim_{A \to \infty} \int_0^A xe^{-x} dx$$

and try various values for A. For example

A	I
1	0.26424
10	0.9995006008
20	0.9999999567157739
100	1.00000000
∞	1.0000000

Multiple integrals

If the limits of integrations are constants then we can sequentially apply one of the previous integration methods

$$\int_A\int f(x,y)dA = \int_a^b \left(\int_c^d f(x,y)dy\right) dx = \int_c^d \left(\int_a^b f(x,y)dx\right) dy$$

If for example we use 4 points in the x direction and 5 in the y direction we can use the trapezoidal rule in the x direction and Simpson's rule in the y direction. This can be written as:

$$\begin{aligned}\int f(x,y)dxdy &= \sum_{j=1}^{m} v_j \sum_{i=1}^{n} w_i f_{ij} \\ &= \frac{\Delta y}{3}\frac{\Delta x}{2}\left[(f_{11}+2f_{21}+2f_{31}+f_{41}) + 4\left(f_{12}+2f_{22}+2f_{32}+f_{42}\right)\right. \\ &\left. + \cdots + (f_{15}+2f_{25}+2f_{35}+f_{45})\right]\end{aligned}$$

Exercises on Multiple integrals

Try the following example:

$$\int_0^1 \left(\int_0^2 xy^2 dx \right) dy = \frac{2}{3}$$

$$\int_0^1 \left(\int_{2y}^2 xy^2 dx \right) dy = \frac{4}{15}$$

$$\int_0^2 \left(\int_0^{x/2} xy^2 dy \right) dx = ?$$