Numerical Integration

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Numerical Integration

Statement of the problem:

Let f be a real function defined on an interval $[a, b]$. We want to determine an approximation of the definite integral

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

Why to provide an approximation:

- It is not always possible to express the primitive of f in terms of elementary functions.
- The function to be integrated may not be given in an analytical form but as a set of points.

Suppose we know (or can evaluate) the integrand function $f(x)$ at points x_i (chosen or predetermined), distinct within the interval $[a, b]$.

$$I(a, b; f) = \int_a^b f(x)\, dx \approx I_n = \sum_{i=0}^{n} c_i f(x_i),$$

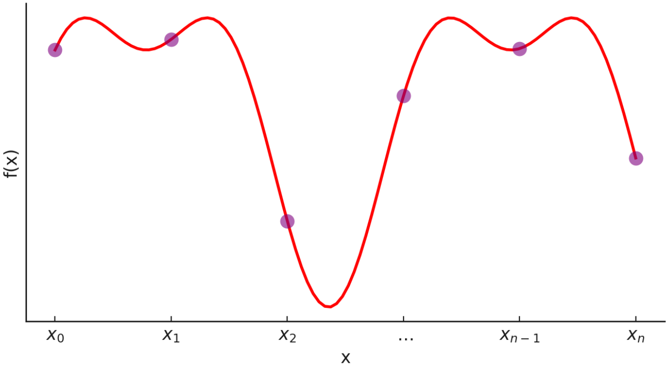
where c_i are weights/coefficients and $f(x_i)$ are the function values on the points x_i
The rest of the quadrature formula is:

$$r_n = I - I_n$$

Numerical integration

A quadrature formula is a weighted sum of function values at appropriate points:

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + \cdots + c_n f(x_n)$$

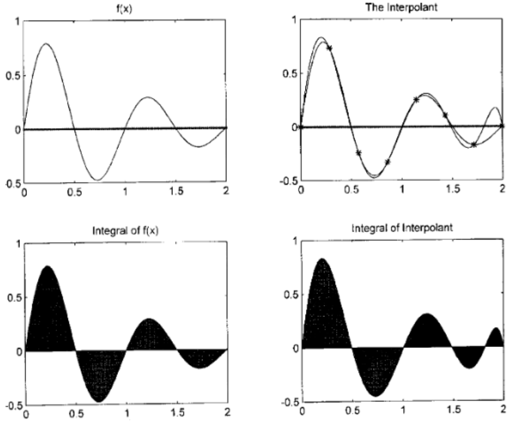


Interpolatory formulas

Idea: The idea is to replace the integrand function, $f(x)$, with a function that is easier to integrate, typically a polynomial.

$$I(a,b;f) = \int_a^b f(x)\,dx \quad I_n(a,b;f) = \int_a^b p_n(x)\,dx$$

where $p_n(x)$ is the polynomial that interpolates $f(x)$ at $n+1$ points $(x_i,\ f(x_i))$



Interpolatory formulas

Let $p_n(x)$ be the Lagrange interpolating polynomial at $n+1$ distinct points.

$$p_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x)$$

$$I_n(f) = \int_a^b p_n(x)dx = \sum_{i=0}^{n} \underbrace{\int_a^b L_i(x)dx}_{c_i} f(x_i)$$

A quadrature formula I_n has a accuracy degree k if it is exact $(r_n = 0)$ when the integrand function is any polynomial $p(x)$ of degree less than or equal to k.

$$I(p) = I_n(p) \quad \forall p \in \mathbb{P}_k$$

The quadrature formula is exact by construction for polynomials of degree at least n (accuracy degree at least n).

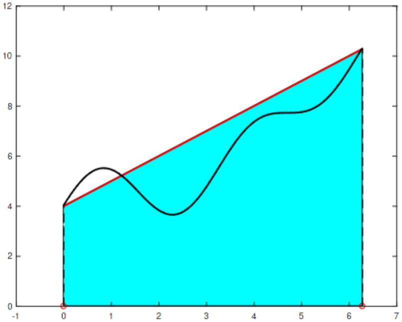
Trapezoidal Rule

Let us consider a linear approximation of $f(x)$

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{1} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1)$$

$$= \frac{h}{2}\left[f(x_0) + f(x_1)\right]$$

where $a = x_0$ and $b = x_1$



Trapezoidal Rule

Lagrange Polynomial, $n = 1$

$$p(x) = L_0(x)f(x_0) + L_1(x)f(x_1)$$

$$p(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

Variable change

$$\xi = \frac{x - x_0}{x_1 - x_0} \in [0, 1], \quad d\xi = \frac{dx}{h}; \quad h = x_1 - x_0$$

$$x = x_0 \implies \xi = 0 \quad \text{and} \quad x = x_1 \implies \xi = 1$$

$$p(\xi) = (1 - \xi)f(a) + \xi f(b)$$

Integrating

$$\int_a^b f(x)dx \approx \int_a^b p(x)dx = h \int_0^1 p(\xi)d\xi$$

$$= f(a)h \int_0^1 (1 - \xi)d\xi + f(b)h \int_0^1 \xi d\xi$$

$$= f(a)h \left(\xi - \frac{\xi^2}{2} \right) \Big|_0^1 + f(b)h \frac{\xi^2}{2} \Big|_0^1 = \frac{h}{2} [f(a) + f(b)]$$

Trapezoidal Rule: an example

Let us calculate the following integral

$$\int_0^4 xe^{2x} dx$$

Exact Solution

$$\int_0^4 xe^{2x} dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4$$

$$= \frac{1}{4}e^{2x}(2x-1)\Big|_0^4 = 5216.926477$$

Trapezoidal Rule

$$I = \int_0^4 xe^{2x} dx \approx \frac{4-0}{2}\left[f(0)+f(4)\right] = 2(0+4e^8) = 23847.66$$

Relative error

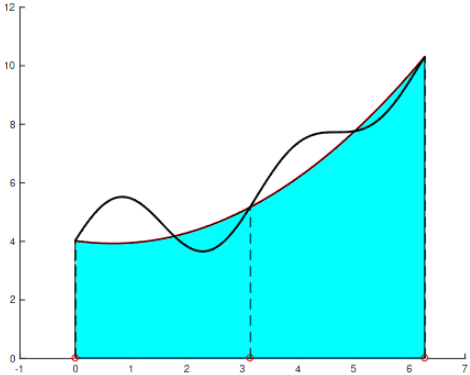
$$\varepsilon = \frac{5216.926 - 23847.66}{5216.926} = -357.12\%$$

Simpson rule 1/3

Let us approximate the function $f(x)$ with a parabola $p(x)$, $n = 2$

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{2} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2)$$

$$= \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$



Simpson rule 1/3

$$p(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)$$

$$\xi = \frac{x-x_1}{h} \in [-1,1], \quad d\xi = \frac{dx}{h}, \quad h = \frac{x_2-x_0}{2}$$

$$\begin{cases} x = x_0 \implies \xi = -1 \\ x = x_1 \implies \xi = 0 \\ x = x_2 \implies \xi = 1 \end{cases}$$

$$p(\xi) = \frac{\xi(\xi-1)}{2} f(x_0) + (1-\xi^2) f(x_1) + \frac{\xi(\xi+1)}{2} f(x_2)$$

$$\int_a^b f(x)dx \approx h \int_{-1}^{1} p(\xi) d\xi =$$

$$= f(x_0)\frac{h}{2}\int_{-1}^{1} \xi(\xi-1)d\xi + f(x_1)h\int_{-1}^{1}(1-\xi^2)d\xi + f(x_2)\frac{h}{2}\int_{-1}^{1}\xi(\xi+1)d\xi$$

$$= f(x_0)\frac{h}{2}\left(\frac{\xi^3}{3} - \frac{\xi^2}{2}\right)\Big|_{-1}^{1} + f(x_1)h\left(\xi - \frac{\xi^3}{3}\right)\Big|_{-1}^{1} + f(x_2)\frac{h}{2}\left(\frac{\xi^3}{3} + \frac{\xi^2}{2}\right)\Big|_{-1}^{1}$$

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

Simpson rule 3/8

Let us approximate the function f(x) with a cubic polynomial, $n = 3$

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{3} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$

$$= \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]$$

Simpson rule 3/8

Calculate the Integral

$$\int_0^4 xe^{2x}dx$$

- **Simpson 1/3**

$$I = \int_0^4 xe^{2x}dx \approx \frac{h}{3}\left[f(0) + 4f(2) + f(4)\right]$$

$$= \frac{2}{3}\left[0 + 4(2e^4) + 4e^8\right] = 8240.411$$

$$\varepsilon = \frac{5216.926 - 8240.411}{5216.926} = -57.96\%$$

- **Simpson 3/8**

$$I = \int_0^4 xe^{2x}dx \approx \frac{3h}{8}\left[f(0) + 3f\left(\frac{4}{3}\right) + 3f\left(\frac{8}{3}\right) + f(4)\right]$$

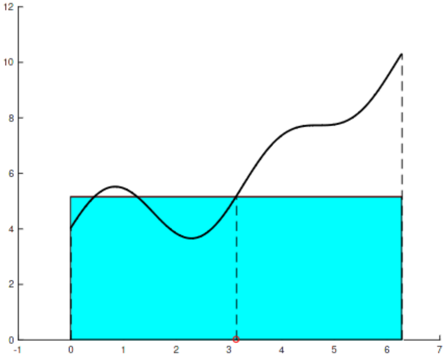
$$= \frac{3(4/3)}{8}\left[0 + 3(19.18922) + 3(552.33933) + 11923.832\right] = 6819.209$$

$$\varepsilon = \frac{5216.926 - 6819.209}{5216.926} = -30.71\%$$

Mid point rule

Let us approximate the function f(x) with a constant function, $n = 0$

$$\int_a^b f(x)dx \approx (x_2 - x_0) f(x_{mid}) \approx (x_2 - x_0) f\left(\frac{x_0 + x_2}{2}\right)$$



Truncation Error

Theorem (Interpolation Error, Cauchy (1840))

Let $f \in C^{n+1}([a,b])$ and suppose that $x_0, \ldots, x_n \in [a,b]$ are distinct, and that the polynomial p_n satisfies

$$p_n(x_k) = f(x_k), \quad k = 0, \ldots, n.$$

Then

$$E_n[f](x) := f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i),$$

where $\xi \in I$ with I being the smallest open interval containing $x_0, \ldots, x_n$.

So we have that the rest of the quadrature formula is given by

$$r_n = \frac{1}{(n+1)!} f^{(n+1)}(\xi) \int_a^b \Pi_n(x) dx$$

where $\Pi_n(x) = \prod_{i=0}^{n} (x - x_i)$

Truncation Error

Since the nodes x_i are equally spaced, the rest expression simplifies as follows

- **If** n is even and $f \in C^{n+2}([a, b])$ then

$$r_n = \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)dt$$

- **If** n is odd and $f \in C^{n+1}([a, b])$ then

$$r_n = \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n))dt$$

Then the Newton-Cotes formulas have an accuracy degree of

$n+1$ **if** n **is EVEN and** n **if** n **is ODD**.

- An example: truncation error for the trapezoidal rule

$$r_1 = \frac{h^3}{2!} f^{(2)}(\eta) \int_0^1 t(t-1)dt$$

$$\int_0^1 t(t-1)dt = \left[\frac{t^3}{3} - \frac{t^2}{2}\right]_0^1 = -\frac{1}{6}$$

$$r_1 = -\frac{1}{12} h^3 f^{(2)}(\xi)$$

Errors in Newton-Cotes Formulas

- **Trapezoidal Rule:**

$$r_1 = -\frac{h^3}{12} f^{(2)}(\xi) \quad h = b - a$$

- **Simpson's 1/3 Rule:**

$$r_2 = -\frac{h^5}{90} f^{(4)}(\xi) \quad h = \frac{b-a}{2}$$

- **Simpson's 3/8 Rule:**

$$r_3 = -\frac{3h^5}{80} f^{(4)}(\xi) \quad h = \frac{b-a}{3}$$

- **Midpoint Rule:**

$$r_0 = -\frac{h^3}{3} f^{(2)}(\xi) \quad h = \frac{b-a}{2}$$

Composite Formulas

- Subdivision of the integration interval $[a, b]$ into N parts

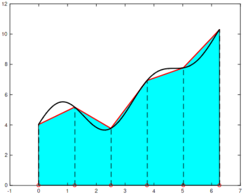
$$[x_i, x_{i+1}], \quad i = 0, 1, \ldots, N-1$$

- Elementary interpolatory formula on each subinterval

$$\int_{x_i}^{x_{i+1}} f(x)dx \quad \text{replaced by} \quad \int_{x_i}^{x_{i+1}} p(x)dx$$

- Sum of integrals over each subinterval

$$\int_a^b f(x)dx = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x)dx$$



Composite Trapezoidal Rule

Let use compute the following integral

$$\boxed{I = \int_0^4 xe^{2x}\, dx}$$

$$N = 1, h = 4 \Rightarrow I = \frac{h}{2}\left[f(0) + f(4)\right] = 23847.66 \quad \varepsilon = -357.12\%$$

$$N = 2, h = 2 \Rightarrow I = \frac{h}{2}\left[f(0) + 2f(2) + f(4)\right] = 12142.23 \quad \varepsilon = -132.75\%$$

$$N = 4, h = 1 \Rightarrow I = \frac{h}{2}[f(0) + 2f(1) + 2f(2)$$
$$+2f(3) + f(4)] = 7288.79 \quad \varepsilon = -39.71\%$$

$$N = 8, h = 0.5 \Rightarrow I = \frac{h}{2}[f(0) + 2f(0.5) + 2f(1)$$
$$+ 2f(1.5) + 2f(2) + 2f(2.5)$$
$$+ 2f(3) + 2f(3.5) + f(4) \quad = \quad 5764.76 \quad \varepsilon \quad = \quad -10.50\%$$

$$N = 16, h = 0.25 \Rightarrow I = \frac{h}{2}[f(0) + 2f(0.25) + 2f(0.5) + \dots$$
$$+2f(3.5) + 2f(3.75) + f(4)] = 5355.95 \quad \varepsilon = -2.66\%$$

Errors in Composite Formulas

- **Trapezoidal Rule:**

$$r_1 = -\frac{b-a}{12} h^2 f^{(2)}(\xi) \quad h = \frac{b-a}{N}$$

- **Simpson's 1/3 Rule:**

$$r_2 = -\frac{b-a}{180} \left(\frac{h}{2}\right)^4 f^{(4)}(\xi) \quad h = \frac{b-a}{N}$$

- **Midpoint Rule:**

$$r_0 = -\frac{b-a}{24} h^2 f^{(2)}(\xi) \quad h = \frac{b-a}{N}$$

The accuracy degree of the composite formulas is the same of the corresponding simple ones but, if $N > 1$, then the step size h is smaller.

Some Numerical Comparisons

Example.
Approximate the definite integral

$$I = \int_0^1 x^3\sqrt{x}\,dx = \frac{2}{9},$$

using the known composite formulas for $N = 1, 2, 4, \ldots,$.

Some Numerical Comparisons

N	$(r_0^{(c)}(f))_N$	$(r_1^{(c)}(f))_N$	$(r_2^{(c)}(f))_N$
1	3.76	3.86	14.56
2	3.93	3.96	15.00
4	3.98	3.99	15.31
8	4.00	4.00	15.53
16	4.00	4.00	15.67
32	4.00	4.00	15.77
64	4.00	4.00	15.84
128	4.00	4.00	15.88
256	4.00	4.00	15.92
512	4.00	4.00	16.06

Table: Error decay for the composite rectangle, trapezoidal, and Cavalieri-Simpson formulas, for N subintervals, in calculating $I = \int_0^1 x^3 \sqrt{x} dx$. Ratios between two successive errors are shown for each formula.

Some Numerical Comparisons

Example.

Approximate the definite integral

$$I = \int_0^1 \sqrt{x}\, dx = \frac{2}{3},$$

using the known composite formulas for $N = 1, 2, 4, \ldots, 1024$.

Unlike the previous case, the convergence of the three families of formulas is very slow. This is mainly due to the fact that although the function is continuous in $[a, b]$, it does not even belong to $C^1[0, 1]$ since it is not differentiable at 0.

Nevertheless, the formulas still converge.

Some Numerical Comparisons

N	$(r_0^{(c)}(f))_N$	$(r_1^{(c)}(f))_N$	$(r_2^{(c)}(f))_N$
1	2.47	2.64	2.82
2	2.59	2.70	2.83
4	2.67	2.74	2.83
8	2.72	2.77	2.83
16	2.75	2.79	2.83
32	2.78	2.80	2.83
64	2.80	2.81	2.83
128	2.80	2.81	2.83
256	2.81	2.82	2.83
512	2.82	2.82	2.83
1024	2.82	2.82	2.83

Table: Error decay for the composite rectangle, trapezoidal, and Cavalieri-Simpson formulas, for N subintervals, in calculating $I = \int_0^1 \sqrt{x}dx$. Ratios between two successive errors are shown for each formula.

Gaussian Quadrature Formulas

Newton-Cotes Formulas

- Use values of the function at $n+1$ equally spaced nodes.
- Degree of precision n (if n is odd) or $n+1$ (if n is even)
- n is the degree of polynomial interpolation.

Question: What are the coefficients c_i and nodes x_i such that the quadrature formula

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} c_i f(x_i)$$

is exact for a polynomial of the highest possible degree?

Gaussian Formulas

- The nodes $x_0, x_1, \ldots$ are not predefined; nodes and coefficients are determined to maximize the degree of precision.

Gaussian Quadrature Formulas: Method of Undetermined Coefficients

- $n = 1: \quad \int_{-1}^{1} f(x)\,dx = c_0 f(x_0) + c_1 f(x_1)$
- Exact formula for $f = x^0, x^1, x^2, x^3$
- Non-linear system of 4 equations and 4 unknowns

$$
\begin{aligned}
f = 1 \quad &\Rightarrow \quad \int_{-1}^{1} 1\,dx = 2 = c_0 + c_1 \\
f = x \quad &\Rightarrow \quad \int_{-1}^{1} x\,dx = 0 = c_0 x_0 + c_1 x_1 \\
f = x^2 \quad &\Rightarrow \quad \int_{-1}^{1} x^2\,dx = \frac{2}{3} = c_0 x_0^2 + c_1 x_1^2 \\
f = x^3 \quad &\Rightarrow \quad \int_{-1}^{1} x^3\,dx = 0 = c_0 x_0^3 + c_1 x_1^3
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
c_0 &= 1 \\
c_1 &= 1 \\
x_0 &= -\frac{1}{\sqrt{3}} \\
x_1 &= \frac{1}{\sqrt{3}}
\end{aligned}
$$

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

- Degree of precision: $2n + 1 = 3$

Gauss-Legendre Formulas

- Alternatively, the nodes of a Gaussian formula are obtained using orthogonal polynomials. The nodes are the roots of orthogonal polynomials with respect to appropriate weight functions $w(x) \geq 0$ in $[a, b]$:

$$\boxed{\int_a^b w(x) f(x)\, dx \approx \sum_{i=0}^{n} c_i f(x_i)}$$

where $c_i = \int_a^b w(x) L_i(x)$

$$n = 1: \quad \text{interval } [-1, 1]; \quad w(x) = 1$$

$$p_0(x) = 1; \quad p_1(x) = x;$$

$$p_2(x) = \frac{1}{2}(3x^2 - 1), \quad \text{with roots } x_0 = -\frac{1}{\sqrt{3}},\, x_1 = \frac{1}{\sqrt{3}},$$

Determine c_0 and c_1 such that the formula is exact for polynomials of degree $< n + 1$

Example

- **Calculate** $I = \int_0^4 te^{2t}dt = 5216.926477$
- **Coordinate Transformation**

$$t = \frac{b-a}{2}x + \frac{b+a}{2} = 2x + 2; \quad dt = 2dx$$

$$I = \int_0^4 te^{2t}dt = \int_{-1}^{1} (4x+4)e^{4x+4}dx = \int_{-1}^{1} f(x)dx$$

- **Gaussian Quadrature Formula for 2 points**

$$I = \int_{-1}^{1} f(x)dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

$$= (4 - \frac{4}{\sqrt{3}})e^{4-\frac{4}{\sqrt{3}}} + (4 + \frac{4}{\sqrt{3}})e^{4+\frac{4}{\sqrt{3}}}$$

$$= 9.167657324 + 3468.376279 = 3477.543936 \quad (\varepsilon = 33.34\%)$$

Gaussian Quadrature Formulas

$$n = 2: \quad \int_{-1}^{1} f(x)dx = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2)$$

Choose $(c_0, c_1, c_2, x_0, x_1, x_2)$ in order to maximize the degree of precision, that is, to impose that the integral is "exact" for $f(x) = x^0, x^1, x^2, x^3, x^4, x^5$

Gaussian Quadrature Formulas: Method of Indeterminate Coefficients

$$
\begin{aligned}
f = 1 \quad &\Rightarrow \int_{-1}^{1} 1 dx = 2 = c_0 + c_1 + c_2 \\
f = x \quad &\Rightarrow \int_{-1}^{1} x dx = 0 = c_0 x_0 + c_1 x_1 + c_2 x_2 \\
f = x^2 \quad &\Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_0 x_0^2 + c_1 x_1^2 + c_2 x_2^2 \\
f = x^3 \quad &\Rightarrow \int_{-1}^{1} x^3 dx = 0 = c_0 x_0^3 + c_1 x_1^3 + c_2 x_2^3 \\
f = x^4 \quad &\Rightarrow \int_{-1}^{1} x^4 dx = \frac{2}{5} = c_0 x_0^4 + c_1 x_1^4 + c_2 x_2^4 \\
f = x^5 \quad &\Rightarrow \int_{-1}^{1} x^5 dx = 0 = c_0 x_0^5 + c_1 x_1^5 + c_2 x_2^5
\end{aligned}
$$

$$
I = \int_{-1}^{1} f(x)\, dx = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)
$$

- $2n + 1 = 5$

Example

$$I = \int_0^4 te^{2t}dt = \int_{-1}^{1} (4x+4)e^{4x+4}dx = 5216.926477$$

Formula with three points $n = 3$:

$$I = \int_{-1}^{1} f(x)dx = \frac{5}{9} f\left(-\sqrt{0.6}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{0.6}\right)$$

$$= \frac{5}{9}\left(4 - 4\sqrt{0.6}\right) e^{4-\sqrt{0.6}} + \frac{8}{9}\left(4e^4\right) + \frac{5}{9}\left(4 + 4\sqrt{0.6}\right) e^{4+\sqrt{0.6}}$$

$$= \frac{5}{9} \times (2.221191545) + \frac{8}{9} \times (218.3926001) + \frac{5}{9} \times (8589.142689)$$

$$= 4967.106689 \quad (\varepsilon = 4.79\%)$$

Formula with four points $n = 4$:

$$I = \int_{-1}^{1} f(x)dx = 0.34785\,[f(-0.861136) + f(0.861136)]$$

$$+\ 0.652145\,[f(-0.339981) + f(0.339981)] = 5197.54375 \quad (\varepsilon = 0.37\%)$$

Gaussian Quadrature Formulas

$$I_{w,f} = \int_a^b w(x)f(x)dx$$

where $w(x)$ is the weight function $w(x) \geq 0$ on $[a, b]$.

Interval	$w(x))$	**Orthogonal polynomials**
$[-1, 1]$	1	Legendre polynomials
$[-1, 1]$	$(1-x)^{\alpha}(1+x)^{\beta}$, $\alpha, \beta > -1$	Jacobi polynomials
$[-1, 1]$	$\frac{1}{\sqrt{1-x^2}}$	Chebyshev polynomials (first kind)
$[-1, 1]$	$\sqrt{1-x^2}$	Chebyshev polynomials (second kind)
$[0, \infty)$	e^{-x}	Laguerre polynomials
$[-\infty, \infty]$	e^{-x^2}	Hermite polynomials

Gaussian Quadrature Formulas

Theorem

$$\int_a^b w(x)f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i) \tag{1}$$

Let $x_0, x_1, \ldots, x_n$ be the zeros of the $n+1$-th orthogonal polynomial $p_{n+1}(x)$ in the interval $[a, b]$ with respect to the weight function $w(x)$.
If the coefficients are determined so that formula (1) is exact for every polynomial of degree less than $n+1$, then the Gaussian quadrature formula (1) has an accuracy degree of $2n+1$.

Proof
Let $f \in \mathbb{P}_{2n+1}$. Let us divide $f(x)$ by p_{n+1}:

$$f(x) = p_{n+1}q + r \quad q, r \in \mathbb{P}_n$$

Consequently $f(x_i) = r(x_i)$, with x_i roots of p_{n+1}:

$$\int_a^b f(x)w(x)dx = \int_a^b (p_{n+1}q + r)w(x)dx = \int_a^b p_{n+1}(x)q(x)w(x)dx + \int_a^b r(x)w(x)dx =$$

$$\sum_{i=0}^{n} w_i r(x_i) = \sum_{i=0}^{n} w_i f(x_i)$$

Convergence of Interpolation Formulas

The convergence of algebraic formulas, obtained by integrating the interpolating polynomial, depends on the family of selected nodes.

- If we consider the Chebyshev nodes $\{x_k^{(ch)}\}_{k=0,\dots,n}$, as seen in polynomial interpolation, we have for the Bernstein theorem that

$$\lim_{n\to\infty} \max_{x\in[a,b]} |f(x) - p_n(x)| = 0, \tag{1}$$

  and we can deduce that

$$\lim_{n\to\infty} \int_a^b p_n(x)\,dx = \int_a^b f(x)\,dx.$$

- On the other hand, if we consider the equispaced nodes $\{x_k^{(e)}\}_{k=0,\dots,n}$, as seen in polynomial interpolation, one cannot affirm that (1) is verified. as can be verified for $f(x) = \frac{1}{1+x^2}$, that is, the Runge function.
- if we consider composite formulas, as seen in polynomial interpolation, the (1) is verified

Convergence of Interpolation Formulas

The family of Newton-Cotes rules does not converge to the required integral, unlike what happens when using interpolation formulas at Chebyshev nodes (as predicted by the theory).

n	E_n^e	E_n^{ch}
10	1.9e+00	1.7e-01
20	3.0e+01	3.3e-03
30	7.7e+02	6.2e-05
40	2.5e+04	1.2e-06
50	8.9e+05	2.1e-08
60	7.3e+09	4.7e-10
70	1.0e+07	2.7e-12
80	6.3e+05	6.1e-13
90	1.4e+05	4.1e-14
100	1.9e+03	4.4e-15

Table: In the first column, the parameter n represents the degree of the interpolating polynomial. In the second and third columns, the absolute quadrature errors are given, obtained by integrating the interpolants at $n+1$ equispaced nodes and Chebyshev nodes in the interval $[-5, 5]$.

Convergence of Composite Formulas

N	$E_0^{(C)}(f)$	$E_1^{(C)}(f)$	$E_2^{(C)}(f)$
1	7.3e+00	2.4e+00	4.0e+00
2	1.4e+00	2.4e+00	9.6e+02
4	4.6e-01	1.4e+01	1.3e-01
8	9.3e-02	3.6e-01	1.5e+00
16	2.1e-04	6.9e-04	9.1e-05
32	1.6e-04	6.6e-04	1.0e-05
64	7.5e-05	6.0e-05	2.6e-09
128	1.3e-06	1.2e-06	4.6e-10
256	5.0e-07	9.8e-07	9.5e-10
512	1.2e-07	3.8e-07	4.4e-10
1024	1.7e-08	2.6e-08	3.7e-11
2048	4.4e-09	3.7e-09	9.4e-12
4096	9.5e-10	9.6e-10	5.3e-13
8192	1.5e-10	1.6e-10	4.0e-14
16384	4.4e-12	1.0e-11	4.4e-16
32768	1.4e-12	3.7e-13	4.0e-17
65536	2.9e-11	5.7e-13	0.0e+00
131072	4.5e-12	3.9e-13	0.0e+00
262144	8.1e-12	2.8e-13	0.0e+00
524288	1.4e-12	1.2e-13	0.0e+00
1048576	1.1e-13	2.2e-13	0.0e+00

Table: Comparison of the composite rectangle, trapezoidal, and Cavalieri-Simpson formulas, for N subintervals, relative to the calculation of $I = \int_{-5}^{5} \frac{1}{1+x^2}\, dx$, where the absolute errors $E_0^{(c)}(f)$, $E_1^{(c)}(f)$, $E_0^{(c)}(r)$, $E_1^{(c)}(r)$ are described for each formula.

Stability of a Quadrature Formula

From

$$S(f) = \sum_{j=1}^{n} c_j f_j, \quad \tilde{S}(f) = \sum_{j=1}^{n} c_j \tilde{f}_j,$$

we derive from the triangular inequality

$$|S(f) - \tilde{S}(f)| = \left| \sum_{j=1}^{n} c_j (f_j - \tilde{f}_j) \right| \leq \sum_{j=1}^{n} |c_j||f_j - \tilde{f}_j|$$

$$\leq \left(\sum_{j=1}^{n} |c_j| \right) \cdot \max_j |f_j - \tilde{f}_j|.$$

Thus, the quantity

$$\sum_{j=1}^{n} |c_j|$$

is an **index of stability** for the quadrature formula S.

Stability of a Quadrature Formula

If the formula has at least degree 0, $\{c_j^+\}_{j=1,\dots,n_+}$ and $\{c_k^-\}_{k=1,\dots,n_-}$ are respectively the positive and negative weights:

$$\int_a^b w(x)dx = \int_a^b 1 \cdot w(x)dx = \sum_{j=1}^{n} c_j = \sum_{j=1}^{n_+} c_j^+ + \sum_{k=1}^{n_-} c_k^-$$

$$= \sum_{j=1}^{n} |c_j| - 2\sum_{k=1}^{n_-} |c_k^-|,$$

from which the stability index $\sum_{j=1}^{n} |c_j|$ satisfies

$$\sum_{j=1}^{n} |c_j| = \int_a^b w(x)dx + 2\sum_{k=1}^{n_-} |c_k^-|.$$

Thus, the presence of negative weights worsens the stability index $\sum_{j=1}^{n} |c_j|$, while if they are all positive, $\sum_{j=1}^{n} |c_j| = \int_a^b w(x)dx$.

Stability of a Quadrature Formula

n	$\mathcal{I}$
0	2.00000e+00
1	2.00000e+00
2	2.00000e+00
3	2.00000e+00
4	2.00000e+00
5	2.00000e+00
6	2.00000e+00
7	2.00000e+00
8	2.90243e+00
9	2.00000e+00
10	6.12959e+00

Table: Stability index $\mathcal{I}(S_n)$ of closed Newton-Cotes formulas with $n+1$ nodes.

On the other hand, the weights of the Gaussian quadrature formulas are all positive.

Quadrature Formulas

- **Newton-Cotes Formulas**
  - Use of function values at $n+1$ equally spaced points
  - Accuracy degree n or $n+1$
  - The weights are positive only for $n \leq 7$
  - May not converge
- **Gaussian Formulas**
  - Accuracy degree $2n+1$
  - The weights are always positive
  - Always convergent as the number of nodes increases