

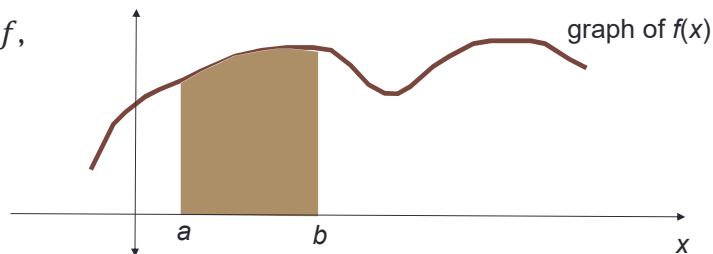
Numerical Computations

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Numerical Integration

For a function f ,



The “integral of f from a to b ” is the area under the graph of the function.

If f is continuous, then the area is well defined, as the common limit of upper and lower sums. The integral is denoted

$$\int_a^b f(x) dx$$

Quadrature formulas with equally-spaced points

Replacing the integrand by some interpolation polynomial, we get the quadrature formulas of the form

$$\int_a^b f(x) dx = \sum_{k=0}^n A_k f(x_k) + E(f)$$

A_k the coefficients depending only on the choice of the points, but not on the form of the function ($k = 0, 1, \dots, n$)

where x_k are the chosen interpolation points

R the remainder term, or the error of the quadrature formula

Quadrature formulas with equally-spaced points (closed type)

The idea is to replace a complicated function with an approximation function that is easy to integrate.

If we know the value of a function, f , at a set of distinct points $\{x_0, \dots, x_n\}$ from the interval $[a, b]$, then the interpolation polynomial

$$P_n(x) = \sum_{i=1}^n f(x_i) L_i(x)$$

is an approximating function for $f(x)$ and its truncation error term over $[a, b]$ is attainable

General Remarks

If the limits of integration a and b are interpolation points, then the formula

$$\int_a^b f(x) dx = \sum_{k=0}^n A_k f(x_k) + E(f)$$

is the *closed type*, otherwise it is called *open type*.

Quadrature formulas with equally-spaced points (closed type)

We have

$$\int_a^b f(x) dx = \int_a^b \sum_{i=1}^n f(x_i) L_i(x) dx + \int_a^b \prod_{i=0}^n (x - x_i) \frac{f^{(n+1)}(\eta(x))}{(n+1)!} dx$$

$$= \sum_{i=1}^n A_i f(x_i) + \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^n (x - x_i) f^{(n+1)}(\eta(x)) dx$$

$$E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^n (x - x_i) f^{(n+1)}(\eta(x)) dx$$

Quadrature formulas with equally-spaced points

(closed type)(Newton-Cotes formulas)

Where $\eta(x) \in [a, b]$ for each x and for each $0 \leq i \leq n$

$$A_i = \int_a^b L_i(x) dx$$

Thus, we have

$$\int_a^b f(x) dx \approx \sum_{i=1}^n A_i f(x_i)$$

With error given by

$$E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^n (x - x_i) f^{(n+1)}(\eta(x)) dx$$

It is shown that the order of error is $\mathcal{O}(h^{2\lfloor \frac{n}{2} \rfloor + 3})$.

Quadrature formulas with equally-spaced points (closed type)

For each $0 \leq i \leq n$

$$A_i = \int_a^b L_i(x) dx,$$

where

$$L_i(x) = \frac{(x - x_0)(x - x_1) \dots (x - x_{i-1})(x - x_{i+1}) \dots (x - x_n)}{(x_i - x_0)(x_i - x_1) \dots (x_i - x_{i-1})(x_i - x_{i+1}) \dots (x_i - x_n)}$$

Let $q = \frac{x - x_0}{h}$. Hence, $x_j = x_0 + jh$ and

$$x - x_j = x - x_0 - jh = qh - jh = (q - j)h$$

for each $1 \leq j \leq n$.

$$\begin{aligned} L_i(x) &= \frac{q(q-1) \dots (q-i+1)(q-i-1) \dots (q-n)}{i \times (i-1) \dots \times 1 \times (-1) \times \dots \times (-1)(n-i)} \\ &= \frac{q(q-1) \dots (q-i+1)(q-i-1) \dots (q-n)}{(-1)^{n-i} i! \times (n-i)!} \end{aligned}$$

Quadrature formulas with equally-spaced points (closed type)

For each $0 \leq i \leq n$

$$L_i(x) = \frac{q(q-1) \dots (q-i+1)(q-i-1) \dots (q-n)}{(-1)^{n-i} i! \times (n-i)!}$$

Let

$$q^{[n+1]} = q(q-1) \dots (q-n)$$

Hence,

$$L_i(x) = \frac{(-1)^{n-i}}{i! \times (n-i)!} \times \frac{q^{[n+1]}}{q-i}$$

And

$$A_i = \int_a^b L_i(x) dx = \frac{(-1)^{n-i}}{i! \times (n-i)!} \int_0^n \frac{q^{[n+1]}}{q-i} (hdq)$$

Quadrature formulas with equally-spaced points (closed type)

For each $0 \leq i \leq n$

$$\begin{aligned} A_i &= h \frac{(-1)^{n-i}}{i! \times (n-i)!} \int_0^n \frac{q^{[n+1]}}{q-i} dq \\ &= (b-a) \times \frac{1}{n} \times \frac{(-1)^{n-i}}{i! \times (n-i)!} \int_0^n \frac{q^{[n+1]}}{q-i} dq \end{aligned}$$

let

$$H_i = \frac{1}{n} \frac{(-1)^{n-i}}{i! \times (n-i)!} \int_0^n \frac{q^{[n+1]}}{q-i} dq$$

Hence, $A_i = (b-a)H_i$. Consequently,

$$\int_a^b f(x) dx \approx \sum_{i=1}^n (b-a)H_i f(x_i)$$

Note that H_i for $0 \leq i \leq n$ is called a Gauss coefficient

Trapezoidal Rule

Let us consider formulas by using first Lagrange polynomial, i.e., for $n = 1$. This gives the Trapezoidal rule.

Let $x_0 = a$, $x_1 = b$ and $h = b - a$

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

Then

$$\begin{aligned} \int_a^b f(x) dx &= \int_{x_0}^{x_1} \left[\frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \right] dx \\ &\quad + \frac{1}{2} \int_{x_0}^{x_1} f''(\eta(x))(x - x_0)(x - x_1) dx \end{aligned}$$

Trapezoidal Rule (cont'd)

Theorem (weighted mean value theorem for integrals).

Suppose that $f(x)$ is differentiable on $[a, b]$ and $g(x)$ is integrable on $[a, b]$ and $g(x)$ does not change sign on $[a, b]$.

Then there exists $c \in (a, b)$ Such that:

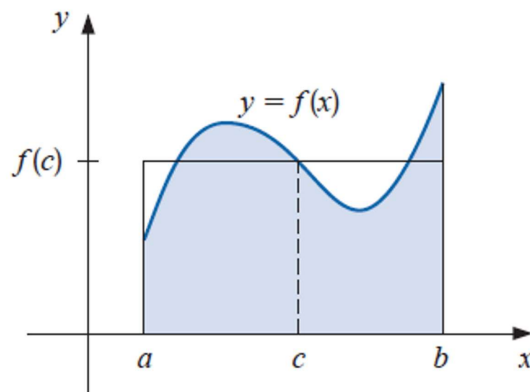
$$\int_a^b f(x)g(x)dx = f(c) \int_a^b g(x)dx$$

When $g(x) \equiv 1$, for some $c \in (a, b)$, we have:

$$f(c) = \frac{1}{b - a} \int_a^b f(x)dx$$

Trapezoidal Rule (cont'd)

We can see it in the following figure:



Trapezoidal Rule (cont'd)

New, we use the above theorem, to calculate the truncation error term:

$$\begin{aligned}
 E(f) &= \int_{x_0}^{x_1} f''(\eta(x))(x - x_0)(x - x_1)dx \\
 &= f''(\eta) \int_{x_0}^{x_1} (x - x_0)(x - x_1)dx \\
 &= f''(\eta) \left[\frac{x^3}{3} - \frac{x_1 + x_0}{2}x^2 + x_0x_1x \right]_{x_0}^{x_1} \\
 &= -\frac{h^3}{3!} f''(\eta)
 \end{aligned}$$

for some $\eta \in (x_0, x_1)$. The order of error is $\mathcal{O}(h^3)$.

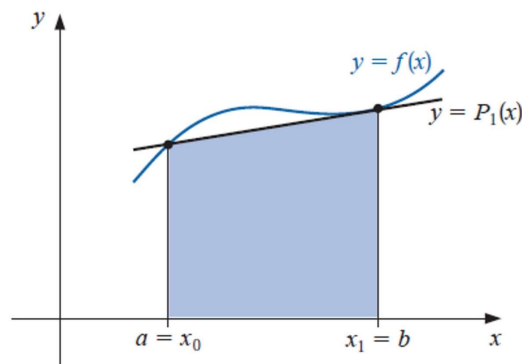
Trapezoidal Rule (cont'd)

Consequently

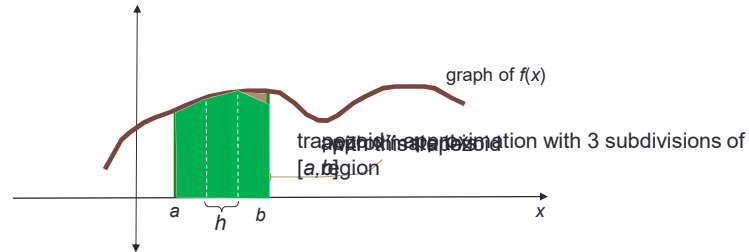
$$\begin{aligned}\int_a^b f(x)dx &= \left[\frac{(x-x_1)^2}{2(x_2-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} \right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\eta) \\ &= \frac{(x_1-x_0)}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\eta) \\ &= \frac{h}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\eta)\end{aligned}$$

Trapezoidal Rule (cont'd)

$$\int_a^b f(x)dx = \frac{h}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f^{(2)}(\eta)$$



Trapezoidal formula



$$\int_a^b f(x) dx \approx h \left(\frac{(f(x_0) + f(x_n))}{2} + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) \right),$$

The remainder term has the form

$$E(f) = -\frac{nh^3}{12} f''(\epsilon) = -\frac{(b-a)h^2}{12} f''(\epsilon), \quad a < \epsilon < b$$

Trapezoidal formula yields the exact value of the integral when the integrand $f(x)$ is a linear function, since we have then $f''(x) = 0$.

Trapezoidal formula (cont'd)

Example: Evaluate the integral $\int_0^1 e^{-x^2} dx$

employing the trapezoidal rule for $n = 10$ and estimate the error of computation.

Solution.

First estimate the remainder term. To this end find the second derivative of the function $y = e^{-x^2}$

$$y'' = 2(2x^2 - 1)e^{-x^2}$$

On the interval $[0, 1]$ the modulus of the second derivative $|y''(x)|$ attains the maximum value at $x = 0$.

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Trapezoidal formula (cont'd)

where $y_i = f(x_i) (i = 0, 1, \dots, 10)$

Example (cont'd).

i	x_i	x_i^2	y_i
0	0	0	1.0000
1	0.1	0.01	0.9900
2	0.2	0.04	0.9608
3	0.3	0.09	0.9139
4	0.4	0.16	0.8521
5	0.5	0.25	0.7788
6	0.6	0.36	0.6977
7	0.7	0.49	0.6126
8	0.8	0.64	0.5273
9	0.9	0.81	0.4449
10	1.0	1.00	0.3679

$$\frac{1}{2}(y_0 + y_{10}) + \sum_{i=1}^9 y_i = 7.4620.$$

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Trapezoidal formula (cont'd)

Example (cont'd).

Thus, we have $y'' = 2(2x^2 - 1)e^{-x^2}$

$$|E(f)| \leq \frac{\max |y''(x)|}{12} |b - a| h^2 = \frac{2 \times (0.1)^2}{12} < 0.002.$$

To remove the effect of the rounding error on the accuracy of the result we shall carry out the computations with one extra digit.
Form a table of values of the integrand function.

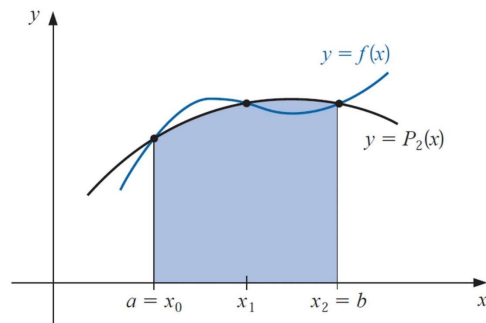
$$\int_0^1 e^{-x^2} dx \approx \frac{1}{10} \left(\frac{1}{2}(y_0 + y_{10}) + \sum_{i=1}^9 y_i \right) = 0.1 \times 7.4620 = 0.7462$$

The final answer is rounded to three digits

$$\int_0^1 e^{-x^2} dx \approx 0.746.$$

Simpson's rule

Suppose that we want to calculate $\int_a^b f(x)dx$ while we know the value of $f(x)$ at $x_0 = a, x_2 = b$ and $x_1 = a + h$ where $h = \frac{b-a}{2}$, i.e., $n = 2$.



Simpson's rule (cont'd)

Therefore

$$\begin{aligned} \int_a^b f(x)dx &= \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) \right. \\ &\quad + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \left. \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \right] dx \\ &\quad + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\eta(x)) dx \end{aligned}$$

Simpson's rule (cont'd)

Therefore

$$H_0 = \frac{1}{2} \cdot \frac{1}{2} \int_0^2 (q-1)(q-2) dq = \frac{1}{4} \left(\frac{8}{3} - 6 + 4 \right) = \frac{1}{6}$$

$$H_1 = -\frac{1}{2} \cdot \frac{1}{1} \int_0^2 q(q-2) dq = \frac{2}{3}$$

$$H_2 = \frac{1}{2} \cdot \frac{1}{2} \int_0^2 q(q-1) dq = \frac{1}{6}$$

$$\begin{aligned} \int_a^b f(x) dx &\approx \sum_{i=1}^2 (b-a) H_i f(x_i) = \frac{h}{3} \sum_{i=1}^2 H_i f(x_i) \\ &= 2h \left(\frac{1}{6} f(x_0) + \frac{2}{3} f(x_1) + \frac{1}{6} f(x_2) \right) \\ &= \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2)) \end{aligned}$$

Simpson's rule (cont'd)

The error:

$$R(h) := E(f) = \int_{x_1-h}^{x_1+h} f(x) dx - \frac{h}{3} (f(x_1-h) + 4f(x_1) + f(x_1+h))$$

For By calculating the error for $n = 1$,

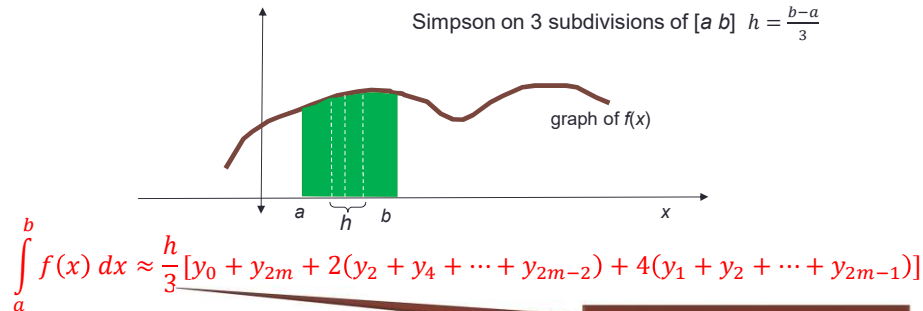
1. $R'(h)$, $R''(h)$ and $R^{(3)}(h)$ are obtained
2. Then by knowing $R(0) = R'(0) = R''(0) = 0$ and mean value theorem, it is obtain

$$3. R(h) = -\frac{h^5}{90} f^{(4)}(\eta) = \mathcal{O}(h^5)$$

Simpson's formula

Simpson on 2 subdivisions of $[a, b]$ $h = \frac{b-a}{2}$

Simpson on 3 subdivisions of $[a, b]$ $h = \frac{b-a}{3}$



where $h = \frac{b-a}{n} = \frac{b-a}{2m}$

The remainder term has the form

$$R_2 = -\frac{mh^5}{90} f^{(4)}(\epsilon) = -\frac{(b-a)h^4}{180} f^{(4)}(\epsilon), \quad a < \epsilon < b$$

- Simpson's formula is exact for polynomials up to degree three, since in this case $f^{(4)}(x) = 0$.
- In Simpson's formula the number of points is obligatory odd, i.e. n is even, $n = 2m$.

Simpson's formula (cont'd)

Example: Evaluate the integral $\int_0^1 e^{x^2} dx$

by Simpson's formula for $n = 10$ and estimate the remainder.

Solution. Estimate the remainder term by finding the fourth derivative of the function $y = e^{x^2}$

$$y^4(x) = 4(4x^4 + 12x^2 + 3)e^{-x^2}$$

The derivative $y^4(x)$ attains the greatest value on the interval $[0, 1]$ at $x = 1$. Thus, we have

$$|R_2| \leq \frac{5 \times (0.1)^5}{90} \times 76 \times 2.718 \approx 0.000115.$$

Form a table of values of the integrand function. Then, applying Simpson's formula, we have:

Simpson's formula (cont'd)

Example (cont'd).

i	x_i	x_i^2	y_i		
			$i = 0, i = 10$	for even i	for odd i
0	0	0	1.0000		
1	0.1	0.01			1.0101
2	0.2	0.04		1.0408	
3	0.3	0.09			1.0942
4	0.4	0.16		1.1735	
5	0.5	0.25			1.2840
6	0.6	0.36		1.4333	
7	0.7	0.49			1.6323
8	0.8	0.64		1.8965	
9	0.9	0.81			1.2479
10	1.0	1.00	2.7183		
Σ			3.7183	5.4441	7.2685

$$\int_0^1 e^{x^2} dx \approx$$

$$\frac{1}{30} (3.7183 + 4 \times 7.2685 + 2 \times 5.4441) = 1.46268,$$

The final answer is rounded to four digits:

$$\int_0^1 e^{x^2} dx \approx 1.4627.$$

Simpson's formula (cont'd)

Example: Evaluate the integral $\int_0^1 \frac{1}{1+x} dx$

by Simpson's formula for $n = 10$ and estimate the remainder.

Solution. Estimate the remainder term by finding the fourth derivative of the function $y = (1+x)^{-1}$

$$f^{(4)}(x) = (-1)(-2)(-3)(-4)(1+x)^{-5} = \frac{24}{(1+x)^5}$$

The derivative $f^{(4)}(x)$ attains the greatest value on the interval $[0, 1]$ at $x = 0$. Thus, we have

$$|R_2| \leq \frac{1 \times (0.1)^4}{180} \times 24 \approx 1.3 \times 10^{-5}$$

Form a table of values of the integrand function. Then, applying Simpson's formula, we have:

Simpson's formula (cont'd)

Example (cont'd).

i	x_i	y_i		
		$i = 0, i = 10$	for even i	for odd i
0	0	1.0000		
1	0.1			0.90909
2	0.2		0.83333	
3	0.3			0.76923
4	0.4		0.71429	
5	0.5			0.66667
6	0.6		0.62500	
7	0.7			0.58824
8	0.8		0.55556	
9	0.9			0.52632
10	1.0	0.50000		
Σ		3.7183	2.72818 σ_2	3.45955 σ_1

$$\int_0^1 \frac{1}{1+x} dx \approx$$

$$\frac{1}{30} (1.50000 + 4 \times 3.45955 + 2 \times 2.72818) = 0.69315,$$

The final answer is rounded to five digits: $\int_0^1 \frac{1}{1+x} dx \approx 0.69315$

Simpson's formula (cont'd)

Solution (cont'd). Let us compute the error of the result which is equal to

$$R_1 = \frac{1}{2} \times 10^{-5}$$

The total error is made up of the error R_1 and R_2 .

Thus, the limiting total error is

$$R = 0.5 \times 10^{-5} + 1.3 \times 10^{-5} = 1.8 \times 10^{-5}$$

Newton's formula ($n = 3$)

$$\text{where } h = \frac{b-a}{3}$$

$$\int_{x_0}^{x_3} f(x) dx \approx \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)],$$

The remainder term has the form

$$R(f) = R_3 = -\frac{3h^5}{80} f^{(4)}(\eta) \quad a < \eta < b$$

Composite Newton's formula ($n = 3$)

$$\text{where } h = \frac{b-a}{n} = \frac{b-a}{2m}$$

$$\int_a^b f(x) dx \approx \frac{3h}{8} [y_0 + y_{3m} + 2(y_3 + y_6 + \cdots + y_{2m-3}) + 3(y_1 + y_2 + y_4 + y_5 + \cdots + y_{2m-2} + y_{2m-1})],$$

The remainder term has the form

$$R_3 = -\frac{3mh^5}{80} f^{(4)}(\eta) = -\frac{(b-a)h^4}{80} f^{(4)}(\eta), \quad a < \eta < b$$

For each n , the remainder term is $\mathcal{O}(h^{2\lfloor \frac{n}{2} \rfloor + 3})$.

Newton's formula (cont'd)

Example: Evaluate the integral

$$\int_0^{0.6} \frac{dx}{1+x}$$

using Newton's formula for $h = 0.1$ and estimate the remainder term.

Solution.

To estimate the remainder term find the fourth derivative of the integrand function $y = (1 + x^{-1})$

$$y^4(x) = 24(1+x)^{-5}$$

On the interval $[0; 0.6]$ it has the greatest value at $x = 0$. Therefore,

$$|R_3| \leq \frac{6 \times (0.1)^5}{80} \times 24 = 1.8 \times 10^{-5}.$$

Newton's formula (cont'd)

Example (cont'd). Form a table of values of the integrand function. Using the results of computations, by Newton's formula we find

i	x_i	$1+x_i$	y_i		
			$i=0, i=6$	$for\ i=3$	$for\ i=1,2,4,5$
0	0	0	1.0000		
1	0.1	0.01			0.90909
2	0.2	0.04			0.83333
3	0.3	0.09		0.76923	
4	0.4	0.16			0.71429
5	0.5	0.25			0.66667
6	0.6	0.36	0.62500		
Σ			1.62500	0.76923	3.12338

$$\int_0^{0.6} \frac{dx}{1+x} \approx \frac{3}{8} \times 0.1(1.62500 + 1.53846 + 9.37014) = 0.47001.$$

Choosing the interval of integration

The problem consists in choosing the interval h to ensure the specified accuracy ε of evaluating the integral by a chosen formula of numerical integration.

Choosing the interval by estimating the remainder term:

Let it be required to evaluate an integral accurate to ε . Using the formula for the corresponding remainder term R , choose h such that the inequality $|R| < \frac{\varepsilon}{2}$ is fulfilled.

Then evaluate the integral by the approximate formula with the interval obtained, the number of digits being such that the rounding error does not exceed $\frac{\varepsilon}{2}$.

Example

Using Simpson's formula evaluate the integral accurate to $\varepsilon = 10^{-3}$.

$$\int_{\frac{\pi}{4}}^{\frac{\pi}{2}} \frac{\sin x}{x} dx$$

Solution.

First choose the interval of integration. The remainder term of Simpson's formula has the form

$$R = -\frac{h^4(b-a)}{180} f^4(\varepsilon), \quad a < \varepsilon < b$$

Choose the interval h so that the following inequality is satisfied

$$\frac{h^4(b-a)}{180} \max_{[a,b]} |f^4(x)| < 0.5 \times 10^{-3}.$$

Example (cont'd)

Compute $f^4(x)$

$$f^4(x) = \frac{\sin x}{x} + 4 \frac{\cos x}{x^2} - 12 \frac{\sin x}{x^3} - 24 \frac{\cos x}{x^4} + 24 \frac{\sin x}{x^5}.$$

In estimating $|f^4(x)|$ on the interval $[\frac{\pi}{2}, \frac{\pi}{4}]$ take advantage of the fact that the quantities are positive and decrease on this interval.

$$\frac{\sin x}{x} \left(1 - \frac{12}{x^2} + \frac{24}{x^4} \right) \text{ and } 4 \frac{\cos x}{x^2} \left(\frac{6}{x^2} - 1 \right).$$

Example (cont'd)

Therefore, they reach and the greatest value at the point $\frac{\pi}{4}$,

$$|f^4(x)| \leq \frac{\sin x}{x} \left(1 - \frac{12}{x^2} + \frac{24}{x^4} \right) + 4 \frac{\cos x}{x^2} \left(\frac{6}{x^2} - 1 \right) < 81.$$

Thus, for determining the interval of computation h we obtain the inequality

$$\frac{h^4 \frac{\pi}{4}}{180} \times 81 < 0.5 \times 10^{-3}$$

whence $h^4 < 14 \times 10^4$ and $h < 1.9 \times 10^{-1} = 0.19$. On the other hand, the spacing h should be chosen so as to into an even number of equal subdivide the interval $[\frac{\pi}{2}, \frac{\pi}{4}]$ into an even number of equal parts. The two mentioned conditions are met by the following values:

$$h = \frac{\pi}{4} = 0.13 < 0.19, \quad n = \frac{(b-a)}{h} = 6$$

Example (cont'd)

To ensure the error not exceeding 0.5×10^{-3} it is sufficient to carry out the computations accurate to four decimal places.

Form a table of values of the function $y = \frac{\sin x}{x}$ with $h = \frac{\pi}{24} = 7^\circ 30' = 0.13090$. the last row containing the results of summation for the last three columns.

Then, using Simpson's formula, we find for $n = 6$:

$$\int_{\frac{\pi}{4}}^{\frac{\pi}{2}} \frac{\sin x}{x} dx \approx \frac{h}{3} [(y_0 + y_6) + 4(y_1 + y_3 + y_5) + 2(y_2 + y_4)].$$

Example (cont'd)

i	x_i°	x_i	$\sin x$	y_0, y_6	y_{2m}	y_{2m-1}
0	45°00'	0.7854	0.7071	0.9003		
1	52°30'	0.9163	0.7934			0.8659
2	60°00'	1.0472	0.8660		0.8270	
3	67°30'	1.1781	0.9239			0.7842
4	75°00'	1.3090	0.9659		0.7379	
5	82°30'	1.4399	0.9914			0.6885
6	90°00'	1.5708	1.0000	0.6366		
Σ				1.5369	1.5649	2.3386

$$\int_{\frac{\pi}{4}}^{\frac{\pi}{2}} \frac{\sin x}{x} dx = 0.043633(1.5369 + 4 \times 2.3386 + 2 \times 1.5649) = 0.6118$$

The final result is rounded to three digits:

$$\int_{\frac{\pi}{4}}^{\frac{\pi}{2}} \frac{\sin x}{x} dx \approx 0.612$$

Choosing the interval of integration

Double computation: Since the finding of $\max |f^{(k)}(x)|$ often involves many cumbersome calculations, the following method is used in computational practice: integral I is evaluated by the chosen quadrature formula twice.

Denoting the results of computation by I_n and I_{2n} , respectively, compare them. If $|I_n - I_{2n}| < \varepsilon$, where ε is the permissible error, then put $I \approx I_{2n}$.

But if it turns out that $|I_n - I_{2n}| \geq \varepsilon$ then the computation is repeated taking the spacing $\frac{h}{4}$. Sometimes a number close to $\sqrt[m]{\varepsilon}$ may be recommended as the initial spacing, where $m = 2$ for the trapezoidal formula and $m = 4$ Simpson's formula.

Note that for an approximate estimate of the truncation error Δ we can use *Runge's principle*, according to which

for the
trapezoidal
formula

$$\Delta \approx \frac{1}{3} |I_n - I_{2n}| < \varepsilon$$

$$\Delta \approx \frac{1}{15} |I_n - I_{2n}| < \varepsilon$$

for
Simpson's
formula

Example

Compute the following integral by Simpson's formula accurate to $\varepsilon = 3 \times 10^{-4}$.

$$\int_0^{\pi} \frac{dx}{x + \cos x}$$

Solution.

Subdivide the interval $[0, \pi]$ into eight parts and find the values of the integrand function at the points of division. Then evaluate the integral by Simpson's formula first for the spacing $h = \frac{\pi}{8}$ ($n = 8$), and then for $h = \frac{\pi}{4}$ ($n = 4$)

Example (cont'd)

i	x_i^2	x_i	$\cos x_i$	$x_i + \cos x_i$	y_i	m'_i	m_i
0	0°	0	1.0000	1.0000	<u>1.0000</u>	1	1
1	22°30'	0.3927	0.9239	1.3166	0.7595	4	
2	45°	0.7854	0.7071	1.4925	<u>0.6700</u>	2	4
3	67°30'	0.1781	0.3827	1.5608	0.6407	4	
4	90°	1.5708	0.0000	1.5708	<u>0.6366</u>	2	2
5	112°30'	1.9635	-0.3827	1.5808	0.6326	4	
6	135°	2.3562	-0.7071	1.6491	<u>0.6064</u>	2	4
7	157°30'	2.7489	-0.9239	1.8250	0.5480	4	
8	180°	3.1416	-1.0000	2.1416	<u>0.4669</u>	1	1
Σ						15.6161	7.8457

Example (cont'd)

By Simpson's formula we find:

For $n = 4, h = \frac{\pi}{4} = 0.78540, h = \frac{\pi}{3} = 0.26180$

$$I_4 = 0.26180 \times 7.8457 = 2.0540;$$

For $n = 8, h = \frac{\pi}{8} = 0.39270, h = \frac{\pi}{3} = 0.13090$

$$I_8 = 0.13090 \times 15.6161 = 2.0441;$$

Comparing the values I_4 and I_8 , we get

$$|I_4 - I_8| = 0.0099 > 3 \times 10^{-4}$$

Moreover, even $\frac{1}{15} |I_4 - I_8| > 3 \times 10^{-4}$, therefore the error of the more accurate value I_8 is still not sufficient. Consequently the spacing should be reduced. Carry out analogous computations with the spacings: $h = \frac{\pi}{8}$ and $h = \frac{\pi}{16}$.

Example (cont'd)

i	x_i^0	x_i	$\cos x_i$	$x_i + \cos x_i$	y_i	m'_i
0	0°	0	1.0000	1.0000	1.0000	1
1	11°15'	0.1963	0.9808	1.1771	0.8495	4
2	22°30'	0.3927	0.9239	1.3166	0.7595	2
3	33°45'	0.5890	0.8315	1.4205	0.7040	4
4	45°	0.7854	0.7071	1.4925	<u>0.6700</u>	2
5	56°15'	0.9817	0.5554	1.5371	0.6506	4
6	67°30'	1.1781	0.3827	1.5608	0.6407	2
7	78°45'	1.3744	0.1951	1.5695	0.6371	4
8	90°	1.5708	0	1.5708	0.6366	2
9	101°15'	1.7670	-0.1951	1.5719	0.6361	4
10	112°30'	1.9635	-0.3827	1.5808	0.6326	2
11	123°45'	2.1599	-0.5554	1.6045	0.6332	4
12	135°	2.3562	-0.7071	1.6491	0.6064	2
13	146°15'	2.5525	-0.8315	1.7210	0.5810	4
14	157°30'	2.7489	-0.9239	1.8250	0.5480	2
15	168°45'	3.9452	-0.9808	1.9644	0.5090	4
16	180°	3.1416	-1.0000	2.1416	0.4669	1
					Σ	31.2169

Example (cont'd)

By Simpson's formula we find:

For $n = 16, h = \frac{\pi}{16} = 0.19635$,

$$I_{16} = 0.06545 \times 31.2169 = 2.0540;$$

Comparing the values I_4 and I_8 , we get

$$|I_8 - I_{16}| = 0.0010.$$

According to Runge's rule, the error of the more accurate value I_{16} does not exceed $\frac{1}{15} 0.0010 < 3 \times 10^{-4}$. Therefore the value I_{16} is computed to the required accuracy. Thus:

$$\int_0^{\pi} \frac{dx}{x + \cos x} = 2.0432.$$

Gaussian Quadrature Formulas



Statue of Gauss at his birthplace,
Brunswick

Gaussian quadrature formulas

Features of a Newton-Cotes Formula:

1. The Newton-Cotes formulas were derived by integrating interpolating polynomials.
2. All the Newton-Cotes formula use values of the function at equally-spaced points.
3. The error term in the interpolating polynomial of degree n involves the $(n + 1)$ st derivative of the function being approximated.
4. So a Newton-Cotes formula is exact when approximating the i. integral of any polynomial of degree less than or equal to n .

Definition. A quadrature rule has degree of precision d if the rule integrates all polynomial of degree d or less exactly.

Gaussian quadrature formulas

In the Gaussian quadrature formulas the coefficients A_i and abscissas $t_i (i = 1, 2, \dots, n)$ are chosen so that the formula be accurate for all the polynomials of the highest possible degree N .

$$\int_{-1}^1 f(t) dt = \sum_{i=1}^n A_i f(t_i) + R_n(f)$$

n	t_i	A_i	$R_n(f)$
4	$-t_1 = t_4 = 0.861136312$ $-t_2 = t_3 = 0.339981044$	$A_1 = A_4 = 0.347854845$ $A_2 = A_3 = 0.652145155$	$R_4(f) \approx 2.88 \times 10^{-7} f^{(8)}(\varepsilon)$ $-1 < \varepsilon < 1$
5	$-t_1 = t_5 = 0.906179846$ $-t_2 = t_4 = 0.538469310$ $t_3 = 0$	$A_1 = A_5 = 0.236926885$ $A_2 = A_4 = 0.478628670$ $A_3 = 0.568888889$	$R_5(f) \approx 8.08 \times 10^{-4} f^{(10)}(\varepsilon)$ $-1 < \varepsilon < 1$
7	$-t_1 = t_7 = 0.949107912$ $-t_2 = t_6 = 0.741531186$ $-t_3 = t_5 = 0.405845151$ $t_4 = 0$	$A_1 = A_7 = 0.129484966$ $A_2 = A_6 = 0.279705391$ $A_3 = A_5 = 0.381830051$ $A_4 = 0.417959184$	$R_7(f) \approx 2.13 \times 10^{-1} f^{(14)}(\varepsilon)$ $-1 < \varepsilon < 1$

Gaussian quadrature formulas (cont'd)

In computing the integral $\int_{-1}^1 f(t) dt = \sum_{i=1}^n A_i f(t_i) + R_n(f)$

The coefficients A_1, \dots, A_n in the approximation formula are arbitrary, and the nodes t_1, \dots, t_n are restricted only by the fact that they must lie in $[-1, 1]$. This gives us $2n$ parameter to choose.

If the coefficients of a polynomial are considered parameters, the class of polynomials of degree at most $2n - 1$ also contains $2n$ parameters. This, then, is the largest class of polynomials for which it is reasonable to expect a formula to be exact. With the proper choice of the values and constants, exactness on this set can be obtained.

Gaussian quadrature formulas (cont'd)

In computing the integral $\int_a^b f(x)dx$

it is advisable to substitute the variable

$$x = \frac{b+a}{2} + \frac{b-a}{2}t$$

then Gauss' formula will have the form

$$\int_a^b f(x)dx = \frac{b-a}{2} \sum_{i=1}^n A_i f(x_i) + R_n^*(f)$$

$$R_n^*(f) = \left(\frac{b-a}{2}\right)^{2n+1} R_n(f)$$

$$x_i = \frac{b+a}{2} + \frac{b-a}{2}t_i$$

Gaussian quadrature formulas for $n = 2$

To illustrate the procedure for choosing the appropriate parameters, we will show how to select the coefficients and nodes when $n = 2$ and the interval of integration is $[-1, 1]$.

$$\int_{-1}^1 f(x)dx \approx A_1 f(t_1) + A_2 f(t_2)$$

gives the exact result whenever $f(x)$ is a polynomial of degree $2(2) - 1 = 3$ or less, that is, when

$$f(x) = a_0 + a_1x + a_2x^2 + a_3x^3,$$

for some collection of constants, a_0, a_1, a_2 , and a_3 . This is equivalent to showing that the formula gives exact results when $f(x)$ is $1, x, x^2$, and x^3 . Hence, we need c_1, c_2, x_1 , and x_2 , so that

Gaussian quadrature formulas for $n = 2$

Hence, we need c_1, c_2, x_1 , and x_2 , so that

$$A_1 \cdot 1 + A_2 \cdot 1 = \int_{-1}^1 1 dx = 2 \quad A_1 \cdot x_1 + A_2 \cdot x_2 = \int_{-1}^1 x dx = 0$$

$$A_1 \cdot x_1^2 + A_2 \cdot x_2^2 = \int_{-1}^1 x^2 dx = \frac{2}{3} \quad A_1 \cdot x_1^3 + A_2 \cdot x_2^3 = \int_{-1}^1 x^3 dx = 0$$

A little algebra shows that this system of equations has the unique solution:

$$A_1 = 1, \quad A_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3}, \quad x_2 = \frac{\sqrt{3}}{3}$$

which gives the approximation formula

$$\int_{-1}^1 f(x) dx \approx A_1 f\left(-\frac{\sqrt{3}}{3}\right) + A_2 f\left(\frac{\sqrt{3}}{3}\right)$$

Example

Compute the integral by Gauss' formula for $n = 5$:

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

Solution.

Substitute the variable

$$x = \frac{1}{2} + \frac{1}{2}t$$

we get the integral

$$I = 2 \int_{-1}^1 \frac{dt}{4 + (t+1)^2}.$$

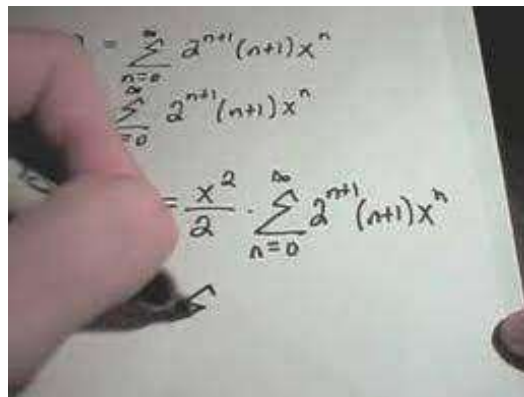
Example (cont'd)

Tabulate the values of the integrand and then find the integral by Gauss' formula for $n = 5$:

i	t_i	$f(t_i)$	A_i
1	-0.906179846	0.24945107	0.236926885
2	-0.538469310	0.23735995	0.478628670
3	0	0.2	0.568888889
4	0.538469310	0.15706261	0.478628670
5	0.906179846	0.13100114	0.236926885

$$I \approx 2[A_1f(t_1) + A_2f(t_2) + A_3f(t_3) + A_4f(t_4) + A_5f(t_5)] \\ = 0.78539816.$$

which is correct for all digits!



$$\begin{aligned} \int \sum_{n=0}^{\infty} a^{n+1}(n+1)x^n &= \sum_{n=0}^{\infty} \int a^{n+1}(n+1)x^n \\ &= \frac{x^2}{2} \cdot \sum_{n=0}^{\infty} a^{n+1}(n+1)x^n \end{aligned}$$

Integrating with
the Aid of
Power Series

Integrating with the aid of power series

Consider the definite integral

$$\int_a^b f(x) dx$$

Let the integrand $f(x)$ be expanded into a power series

$$f(x) = \sum_{k=0}^{\infty} c_k x^k$$

Converging on the interval $(-R, R)$. Applying the theorem on termwise integration of power series, we can represent the integral as a numerical series

$$\int_a^b f(x) dx = \sum_{k=0}^{\infty} \frac{c_k}{k+1} (b^{k+1} - a^{k+1})$$

Integrating with the aid of power series (cont'd)

If the previous series converges sufficiently rapid, then we can compute approximately the definite integral with the aid of the partial sum of the series

$$\int_a^b f(x) dx = \sum_{k=0}^{\infty} \frac{c_k}{k+1} (b^{k+1} - a^{k+1})$$

The error of the final result is made up here of the following errors:

- The error due to the replacement of the series by the partial sum.
- The errors due to rounding off in computing the sum.

Example

Compute the integral $\int_0^1 e^{-x^2}$

by expanding the integrand into a power series and using seven terms of this expansion. Estimate the error.

Solution. We have

$$e^{-x^2} = 1 - x^2 + \frac{x^4}{2!} - \frac{x^6}{3!} + \cdots + (-1)^n \frac{x^{2n}}{n!} + \cdots$$

This series converges for any x ; integrating term wise the first seven terms, we get

$$\begin{aligned} \int_0^1 e^{-x^2} &\approx \left[x - \frac{x^3}{3} + \frac{x^5}{5 \times 2!} - \frac{x^7}{7 \times 3!} + \frac{x^9}{9 \times 4!} - \frac{x^{11}}{11 \times 5!} + \frac{x^{13}}{13 \times 6!} \right]_0^1 \\ &= 1 - \frac{1}{3} + \frac{1}{10} - \frac{1}{42} + \frac{1}{216} - \frac{1}{1320} + \frac{1}{9360}. \end{aligned}$$

Example (cont'd)

Estimating the remainder of the series, we have

$$|R_7| \leq \frac{x^{15}}{15 \times 7!} \Big|_0^1 = \frac{1}{75600} < 1.5 \times 10^{-5}.$$

Taking this into account, we compute the sum to four decimal places. We finally get with all correct digits

$$\int_0^1 e^{-x^2} dx = 0.7468$$

Integrals of Discontinued Functions

The Method of Kantorovich for Isolating Singularities



Leonid Kantorovich
(1912-1986)

Method of Kantorovich for isolating singularities

Suppose it is required to compute the improper integral

$$\int_a^b f(x) dx$$

where the integrand function $f(x)$ turns into infinity at some point c of the interval $[a, b]$. As is known, by definition, we put

$$\int_a^b f(x) dx = \lim_{\substack{\delta_1 \rightarrow 0 \\ \delta_2 \rightarrow 0}} \left\{ \int_a^{c-\delta_1} f(x) dx + \int_{c+\delta_2}^b f(x) dx \right\}$$

To evaluate the converging improper integral to the preassigned accuracy ε choose the positive number δ_1 and δ_2 so small as to fulfill the inequality

$$\left| \int_{c-\delta_1}^{c+\delta_2} f(x) dx \right| < \frac{\varepsilon}{2}.$$

Method of Kantorovich for isolating singularities (c'd)

Then, using some quadrature formulas, we compute approximately the definite integrals

$$S_1 = \int_a^{c-\delta_1} f(x) dx \quad \text{and} \quad S_2 = \int_{c+\delta_2}^b f(x) dx$$

If δ_1 and δ_2 are approximate values of the integrals accurate to $\frac{\varepsilon}{4}$ each, then accurate to ε

$$\int_a^b f(x) dx \approx S_1 + S_2$$

Example

Within 0.05, compute the integral

$$I = \int_{0.3}^2 \frac{e^{-x} dx}{\sqrt[4]{2+x-x^2}}.$$

Solution.

The integrand has a discontinuity at $x = 2$. Let us present the integral as a sum of two integrals

$$I_1 = \int_{0.3}^{2-\delta} \frac{e^{-x} dx}{\sqrt[4]{2+x-x^2}}, \quad I_2 = \int_{2-\delta}^2 \frac{e^{-x} dx}{\sqrt[4]{2+x-x^2}}$$

and choose δ so that the quantity I , turns out to be sufficiently small. For instance, for $\delta \leq 0.1$ the integral I_2 , satisfies the condition

$$0 < I_2 < \frac{e^{-1.9}}{\sqrt[4]{2.9}} \int_{2-\delta}^2 \frac{dx}{\sqrt[4]{2-x}} = 0.115 \times \frac{4}{3} \delta^{\frac{3}{4}} = 0.153 \delta^{\frac{3}{4}},$$

Example (cont'd)

Putting $\delta = 0.1$, we get $I_2 < 0.028$. Taking into account the estimate for the integral I_2 , let us compute

$$I_1 = \int_{0.3}^{2-\delta} \frac{e^{-x} dx}{\sqrt[4]{2+x-x^2}},$$

by Simpson's formula to within 0.022. Computations for the intervals $2h = 0.8$ and $h = 0.4$ yield:

$$I_{1;2h} = 0.519, \quad I_{1;h} = 0.513.$$

Hence, we may write to within 0.004:

$$I_1 \approx 0.51.$$

Thus, putting $I \approx I_1$ we get

$$I \approx 0.51.$$

Method of Kantorovich for isolating singularities (c'd)

Let the integrand function have the form

$$f(x) = (x - c)^\alpha \varphi(x).$$

where $-1 \leq \alpha \leq 0$ and $\varphi(x)$ is continuous and has a sufficient number of derivatives on the interval $[a, b]$.

Example

Calculate the approximate value of the integral

$$I = \int_0^{0.5} \frac{dx}{\sqrt{x(1-x)}}.$$

Solution.

The integrand has a discontinuity at $x = 0$. Let us rewrite it as

$$f(x) = (x - 0)^{-\frac{1}{2}}(1 - x)^{-\frac{1}{2}}$$

Thus $\varphi(x) = (1 - x)^{-\frac{1}{2}}$. By Taylor's formula we have

$$\varphi(x) = 1 + \frac{1}{2}x + \frac{3}{8}x^2 + \frac{5}{16}x^3 + \frac{35}{128}x^4 + R_4(x).$$

Example (cont'd)

Then $f(x)$ can be written in the form

$$f(x) = \left[x^{-\frac{1}{2}} + \frac{1}{2}x^{\frac{1}{2}} + \frac{3}{8}x^{\frac{3}{2}} + \frac{5}{16}x^{\frac{5}{2}} + \frac{35}{128}x^{\frac{7}{2}} \right] + \frac{\psi(x)}{\sqrt{x}}.$$

where

$$\psi(x) = \frac{1}{\sqrt{1-x}} - \left(1 + \frac{1}{2}x + \frac{3}{8}x^2 + \frac{5}{16}x^3 + \frac{35}{128}x^4 \right).$$

and $\psi(0) = 0$.

$$\begin{aligned} I &= \int_0^{0.5} \left(x^{-\frac{1}{2}} + \frac{1}{2}x^{\frac{1}{2}} + \frac{3}{8}x^{\frac{3}{2}} + \frac{5}{16}x^{\frac{5}{2}} + \frac{35}{128}x^{\frac{7}{2}} \right) dx + I_1 \\ &= 1.5691585 + I_1 \end{aligned}$$

$$I_1 = \int_0^{0.5} \frac{\psi(x)}{\sqrt{x}} dx$$

Example (cont'd)

Evaluate the integral I_1 , by Simpson's formula for $n = 10$, i.e. $h = 0.05$.

i	x_i	y_i	m_i
0	0	0.000000	1
1	0.05	0.000000	4
2	0.10	0.000009	2
3	0.15	0.000056	4
4	0.20	0.000216	2
5	0.25	0.000624	4
6	0.30	0.001508	2
7	0.35	0.003225	4
8	0.40	0.006316	2
9	0.45	0.011588	4
10	0.50	0.020239	1
Σ			0.098309

Example (cont'd)

The last row of the table presents the sum of the products of y_i by m_i , whence

$$I_1 = \frac{0.05}{3} \times 0.098309 = 0.0016385$$

we get finally

$$I = \int_0^{0.5} \frac{dx}{\sqrt{x(1-x)}} = 1.5691585 + 0.0016385 = \mathbf{1.5707970}.$$



$$\longrightarrow I = \frac{\pi}{2} = 1.5707963 \approx$$

Applying the weight quadrature formulas (self-study)

Suppose that the function $f(x)$ can be represented in the form of two functions $\varphi(x)$ and $p(x)$:

$$f(x) = \varphi(x)p(x)$$

$\varphi(x)$ being bounded on the interval $[a, b]$ and having a sufficient number of derivatives, while $p(x) > 0$ on $[a, b]$. Then it becomes to chose a quadrature formula of the form

$$\int_{-1}^1 f(x) dx = \int_{-1}^1 \varphi(x)p(x) dx \approx \sum_{k=1}^n C_k^{(n)} \varphi(x_k)$$

Applying the weight quadrature formulas (self-study)

In which the free coefficients $C_k^{(n)}$ are independent of $\varphi(x)$, and the abscissas x_k are determined so that the formula becomes accurate for polynomials of a highest possible degree.

The function $p(x)$ is called the *weight function* or *weight*.

For $a = -1$, $b = 1$ and $p(x) = \frac{1}{\sqrt{1-x^2}}$, there occurs the *Hermitian quadrature formula*.

$$\int_{-1}^1 \frac{\varphi(x) dx}{\sqrt{1-x^2}} = \frac{\pi}{n} \sum_{k=1}^n \varphi(x_k) + R(f),$$

$$x_k = \cos\left(\frac{2k-1}{2n}\pi\right)$$

$$R(f) = \frac{\pi}{(2n)! 2^{n-1}} f^{(2n)}(\varepsilon),$$

$$-1 < \varepsilon < 1$$

Applying the weight quadrature formulas(cont'd) (self-study)

In which the free coefficients $C_k^{(n)}$ are independent of $\varphi(x)$, and the abscissas x_k are determined so that the formula becomes accurate for polynomials of a highest possible degree.

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$$\int_{-1}^1 \frac{\varphi(x) dx}{\sqrt{1-x^2}} = \frac{\pi}{n} \sum_{k=1}^n \varphi(x_k) + R(f),$$

$$x_k = \cos\left(\frac{2k-1}{2n}\pi\right)$$

$$R(f) = \frac{\pi}{(2n)! 2^{n-1}} f^{(2n)}(\varepsilon), \quad -1 < \varepsilon < 1$$

Example (self-study)

Calculate the approximate value of the integral

$$I = \int_{-1}^1 \frac{dx}{\sqrt{1-x^4}}.$$

Solution.

Represent the integrand in the form

$$\frac{1}{\sqrt{1-x^4}} = \frac{1}{\sqrt{1-x^2}} \times \frac{1}{\sqrt{1+x^2}}$$

and consider

$$p(x) = \frac{1}{\sqrt{1-x^2}}$$

as a weight function. Then the given integral can be computed by integral the Hermitian quadrature formula as follows.

Example (cont'd) (self-study)

$$I = \int_{-1}^1 \frac{dx}{\sqrt{1-x^4}} \approx \frac{\pi}{n} \sum_{k=1}^n \frac{1}{\sqrt{1+x_k^2}}.$$

Putting $n = 6$, we get

$$I = \frac{\pi}{6} \left[\frac{2}{\sqrt{1+\cos^2 15^\circ}} + \frac{2}{\sqrt{1+\cos^2 45^\circ}} + \frac{2}{\sqrt{1+\cos^2 75^\circ}} \right]$$

$$= 2.221329$$

Let us note that the direct computation of the integral with six correct digits yields

$$I = 2.221441$$

Applying the weight quadrature formulas (self-study)

Below table contains the values of $C_k^{(n)}$ and x_k for the case when $a = 0$, $b = 1$, and the weight function has the form $p(x) = x^{-\frac{1}{2}}$.

n	k	x_k	$C_k^{(n)}$
3	1	0.056939	0.935828
	2	0.437198	0.721523
	3	0.869499	0.342649
4	1	0.033648	0.725368
	2	0.276184	0.627413
	3	0.634677	0.444762
	4	0.922157	0.202457
5	1	0.022164	0.591048
	2	0.187831	0.538533
	3	0.461597	0.438173
	4	0.748335	0.298903
	5	0.948494	0.133343

Example (self-study)

Calculate the approximate value of the integral

$$I = \int_0^1 \frac{dx}{(4-x)\sqrt{x}}$$

Solution.

Put

$$p(x) = \frac{1}{\sqrt{x}} \quad \varphi(x) = \frac{1}{4-x}$$

Using the values of the above table, we can write

$$I = \int_0^1 \frac{dx}{(4-x)\sqrt{x}} = \frac{0.7254}{3.9664} + \frac{0.6274}{3.7238} + \frac{0.4448}{3.3653} + \frac{0.2025}{3.0778} = 0.5493$$

Direct evaluation of the integral with 4 correct digits yields

$$I = \int_0^1 \frac{dx}{(4-x)\sqrt{x}} = \frac{1}{2} \ln 3 = 0.5493$$

ANY QUESTIONS?