Numerical Methods

Numerical Quadrature

2022-2023

[DΣIM]

Numerical Integration

- We are interested in determining the value of some definite integral of a particular function $f(x)$ within a given interval. This is, we want to compute the value:

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

- The required interval $[a, b]$ does not need to be a finite interval.

Numerical Integration

- Let's suppose that $f(x)$ is an integrable function in the interval $[a, b]$. We are interested in the numerical approximation of the definite integral. This numerical procedure is also known as ***quadrature***. These algorithms are useful when our function is only defined by means of a table, and in the case that there is no primitive function for $f(x)$.

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

Quadrature Formula

- A ***quadrature formula*** is an expression of the form:

$$\int_a^b f(x)dx = F(b) - F(a) \approx \sum_{i=0}^{n} A_i f(x_i)$$

- That will give an approximation of the definite integral of the function $f(x)$ in the domain $[a, b]$ within a certain precision.
- The constants A_i and the interpolation nodes x_i can be chosen using different criteria and provide exact formulae for the integration of polynomials of a given order.

Given abscissas

- This would be the case when our function is defined by means of a table. We may use also an analytic function evaluated in a predetermined set of values of the independent variable x.
- First, we will need to build a partition of the integration interval $[a, b]$:

$$x_0 = a < x_1 < \cdots < x_{n-1} < x_n = b$$

Given abscissas

- Then, we build the classical interpolating polynomial, $P_n(x)$ of the function $f(x)$ using the given set of interpolating nodes: $(x_0, f(x_0)),\ldots.,(x_n, f(x_n))$.
- After that, we can approximate the numerical value of the definite integral by the value of the definite integral of the interpolating polynomial.

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

Newton-Cotes Formulas

- Depending on the degree n of the interpolating polynomial, we can obtain different approximate formulas for the numerical integration. These are known as the ***Newton-Cotes formulas***. If we use the Lagrange polynomial with $n+1$ abscissas, the interpolating polynomial is:

$$P_n(x)=\sum_{k=0}^{n} f(x_k)L_k(x)=\sum_{k=0}^{n} f(x_k)\prod_{i\neq k}\frac{x-x_i}{x_k-x_i}$$

- And the interpolating error is:

$$f(x)=P_n(x)+\frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{k=0}^{n}(x-x_k)$$

Newton-Cotes Formulas

- Then the numerical integral of $f(x)$ can be written as:

$$\int_a^b f(x)dx = \int_a^b \sum_{k=0}^{n} f(x_k)L_k(x)dx + \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{k=0}^{n}(x-x_k)dx$$

$$= \sum_{k=0}^{n} W_k f(x_k) + \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi)\prod_{k=0}^{n}(x-x_k)dx$$

- Where:

$$W_k = \int_a^b L_k(x)dx$$

Newton-Cotes Formulas

- The numerical values W_k are called the ***weights of the integration formula***. These values have the following properties:
- They depend only in the integration interval $[a, b]$ and on the abscissas of the partition. They will never depend on the integrating function $f(x)$
- As the interpolating polynomial is exact for polynomials of certain degree, these formulae will be exact for any polynomial of a degree n or lower.

Newton-Cotes Formulas

- The error in the quadrature can be estimated from the integral:

$$E_n = \int_a^b \big(f(x) - P_n(x) \big)\, dx = \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{k=0}^{n} (x - x_k)\, dx$$

- If the derivatives are bounded within the integration interval $[a, b]$ we can write:

$$\left| E_n \right| \le \frac{M}{(n+1)!} \int_a^b \left| (x - x_0) \cdots (x - x_n) \right| dx$$

The Trapezoidal Rule

- The simplest integration rule is obtained when we use only two abscissas $x_0 = a$ and $x_1 = b$, and we interpolate the function using a straight line.
- In this case the Lagrange interpolating polynomial is simply:

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

The Trapezoidal Rule

- The approximate value of the definite integral is:

$$\int_a^b f(x)dx \approx \int_a^b \left[\frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1) \right] dx$$

$$+\frac{1}{2}\int_a^b f''(\xi)(x-x_0)(x-x_1)dx$$

- We can find an upper bound to the integral error using the mean value theorem in the case of integrals.

The Trapezoidal Rule

- This theorem states that if two given functions $f(x)$ and $g(x)$ are defined within the interval $[a, b]$, being $f(x)$ a continuous function and $g(x)$ integrable with a constant sign within $[a, b]$, then

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

- Being ξ a point in the interval $[a, b]$. Note that the function $(x-a)(x-b)$ does not changes sign within this interval.

The Trapezoidal Rule

- The value of the integral error can be written as:

$$\int_a^b f''(\xi)(x-x_0)(x-x_1)dx = f''(\eta)\int_a^b (x-x_0)(x-x_1)dx$$

$$= f''(\eta)\left[\frac{x^3}{3} - \frac{(x_1+x_0)}{2}x^2 + x_0 x_1 x\right]_{x_0}^{x_1}$$

$$= -\frac{h^3}{6} f''(\eta)$$

- Where we have used the fact that $h = b - a = x_1 - x_0$

The Trapezoidal Rule

- Finally, we obtain the quadrature formula:

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

$$= \left[\frac{(x-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} f(x_1) \right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\eta)$$

$$= \frac{(x_1-x_0)}{2} \left[f(x_0) + f(x_1) \right] - \frac{h^3}{12} f''(\eta)$$

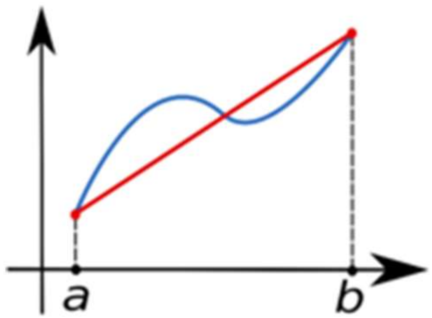
$$= \frac{(b-a)}{2} \left[f(a) + f(b) \right] - \frac{h^3}{12} f''(\eta)$$

The Trapezoidal Rule

- Our first approximation to the definite integral is:

$$\boxed{I(f) = \frac{b-a}{2}\left[f(a) + f(b)\right]}$$

- Which is the expression for the area of trapezoid with basis $(b-a)$ and heights $f(a)$ and $f(b)$



Simpson's Rule

- In this case we will use three evenly spaced abscissas:

$$x_0 = a, \quad x_1 = \frac{a+b}{2}, \quad x_2 = b$$

- To obtain the weights W_k of the formula we can ask alternatively that our quadrature formula should be exact for any polynomials of second degree, that is for the monomials $1, x, x^2$ and then solving the resulting linear system

Simpson's Rule

- We have then

$$b-a=\int_a^b 1dx = W_0+W_1+W_2$$

$$\frac{1}{2}(b^2-a^2)=\int_a^b xdx = aW_0+\frac{a+b}{2}W_1+bW_2$$

$$\frac{1}{3}(b^3-a^3)=\int_a^b x^2dx = a^2W_0+\left(\frac{a+b}{2}\right)^2W_1+b^2W_2$$

Simpson's Rule

- Resulting in the following linear system of equations:

$$\begin{pmatrix} 1 & 1 & 1 \\ a & \dfrac{a+b}{2} & b \\ a^2 & \left(\dfrac{a+b}{2}\right)^2 & b^2 \end{pmatrix} \bullet \begin{pmatrix} W_0 \\ W_1 \\ W_2 \end{pmatrix} = \begin{pmatrix} b-a \\ \dfrac{1}{2}\left(b^2-a^2\right) \\ \dfrac{1}{3}\left(b^3-a^3\right) \end{pmatrix}$$

Simpson's Rule

- Which has the solution:

$$\begin{cases} W_0 = \dfrac{b-a}{6} \\ W_1 = \dfrac{2(b-a)}{3} \\ W_2 = \dfrac{b-a}{6} \end{cases}$$

- Finally, we obtain the quadrature formula

$$I(f) \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

Simpson's Rule

- If we use $h = (b-a)/2$ the formula can be written as

$$\boxed{I(f) \approx \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]}$$

- The error term is in this case:

$$E_2 = \int_a^b \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi)dx$$

Simpson's Rule

- This time, however, it is more convenient to calculate the error as follows.
- Using the Taylor series of $f(x)$ around the middle point x_1 we have:

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2!}(x - x_1)^2$$

$$+ \frac{f^{(3)}(x_1)}{3!}(x - x_1)^3 + \frac{f^{(4)}(\xi)}{4!}(x - x_1)^4$$

Simpson's Rule

- Integrating this expression we have:

$$\int_a^b f(x)dx = f(x_1)(x_2 - x_0) +$$

$$+\left[\frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 + \frac{f^{(3)}(x_1)}{24}(x-x_1)^4\right]_{x_0}^{x_1}$$

$$+\frac{1}{24}\int_a^b f^{(4)}(\xi)(x-x_1)^4 dx$$

Simpson's Rule

- As $(x - x_1)^4$ is not changing sign within $[a, b]$, we can use the mean value theorem for integrals to obtain

$$\frac{1}{24}\int_a^b f^{(4)}(\xi)(x-x_1)^4\,dx = \frac{f^{(4)}(\eta)}{24}\int_a^b (x-x_1)^4\,dx$$

$$= \frac{f^{(4)}(\eta)}{120}\left[(x-x_1)\right]_a^b$$

Simpson's Rule

- Now, as $h = (x_2 - x_1) = (x_1 - x_0)$, we have:

$$(x_2 - x_1)^2 - (x_0 - x_1)^2 = h^2 - (-h)^2 = 0$$

$$(x_2 - x_1)^4 - (x_0 - x_1)^4 = h^4 - (-h)^4 = 0$$

- And:

$$(x_2 - x_1)^3 - (x_0 - x_1)^3 = h^3 - (-h)^3 = 2h^3$$

$$(x_2 - x_1)^5 - (x_0 - x_1)^5 = h^5 - (-h)^5 = 2h^5$$

Simpson's Rule

- The integral value is then

$$\int_a^b f(x)dx = 2hf(x_1) + \frac{h^3}{3} f''(x_1) + \frac{f^{(4)}(\xi)}{60} h^5$$

- Substituting the value of $f''(\xi)$ by a centred formula for the numerical derivation with his associated error we obtain the expression that we can find in the next page.

Simpson's Rule

$$\int_a^b f(x)dx = 2hf(x_1)$$

$$+\frac{h^3}{3}\left[\frac{1}{h^2}\left(f(x_0)-2f(x_1)+f(x_2)\right)-\frac{h^2}{12}f^{(4)}(\xi_1)\right]$$

$$+\frac{f^{(4)}(\xi_2)}{60}h^5$$

$$=\frac{h^3}{3}\left(f(x_0)+4f(x_1)+f(x_2)\right)-\frac{h^5}{12}\left[\frac{f^{(4)}(\xi_1)}{3}-\frac{f^{(4)}(\xi_2)}{5}\right]$$

Simpson's Rule

- The error depends now on the fourth derivative of the function. Thus, the Simpson's Rule will be exact for computing the integrals of polynomials of third degree as is the case for:

$$\int_a^b x^3 dx = \frac{b-a}{6}\left[a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right] = \frac{b^4 - a^4}{4}$$

Exactness Degree

- ***Exactness Degree**:* Given an integration formula its exactness degree is the positive integer such that the error when integrating polynomials of degree $k \leq n$ is $E(P_k) = 0$, while $E(P_{k+1}) \neq 0$.
- Whit this definition the Trapezium rule has an exactness degree of $n = 1$, while Simpson's Rule has an exactness degree of $n = 3$.

Exactness Degree

- We can compare the two rules in the following table, where we have integrated numerically some functions within the interval [0,2]

$f(x)$	x^2	x^4	$1/(x+1)$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact	2.667	6.400	1.099	2.958	1.416	6.389
Trapezium	4.000	16.000	1.333	3.326	0.909	8.389
Simpson	2.667	6.667	1.111	2.964	1.425	6.421

Newton-Côtes Formulae

- The same procedure used for interpolating polynomials of degrees $m = 1$ and $m = 2$, could also be used for higher degrees and obtain the rest of quadrature formulae which receive the generic name of Newton-Côtes formulae.
- Let us work with the following notation: $x_k = x_0 + kh$ where $h = (b - a)/m,$ and m is the degree of the interpolating polynomial, $m + 1$ the number of equidistant nodes, and use $f_k = f(x_k) = f(x_0 + kh)$ for the values of the function.

Newton-Côtes Formulae

- We have then:
- ***Rule 3/8 from Simpson*** (degree n=3):

$$\boxed{\int_a^b f(x)dx = \frac{3h}{8}\left(f_0 + 3f_1 + 3f_2 + f_3\right) - \frac{3h^5}{80} f^{(4)}(\xi)}$$

- ***Boole's Rule*** (degree n=5):

$$\boxed{\int_a^b f(x)dx = \frac{2h}{45}\left(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4\right) - \frac{8h^7}{945} f^{(6)}(\xi)}$$

Composite Formulae

- The Newton-Côtes formulae are ***not a good solution*** for computing integrals within very large intervals.
- Using interpolating polynomials of higher degree will not solve the problem. The degree of the classical interpolating polynomial used, cannot be too high, otherwise we could have to cope with the Runge phenomenon and the oscillatory nature of all polynomials, which will spoil our quadrature.

Composite Trapezium

- What we could do instead, is to divide the interval $[a, b]$ in N equal subintervals using $N+1$ abscissas. Within each subinterval, we could use the trapezium formula and then add up all the results for each interval. This is the ***composite trapezium*** formula.
- First, we divide the integral as

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

Composite Trapezium

- Where we are using the abscissas $x_k = a + kh,\ k = 0,1,\dots,N$. The size of each subinterval is:

$$h = \frac{b-a}{N}$$

- If now, we use the notation:

$$I_k(f) = \int_{x_k}^{x_{k+1}} f(x)dx$$

Composite Trapezium

- And we apply the Trapezium rule to compute each of the $I_k(f)$, we have

$$I_k(f) = \int_{x_k}^{x_{k+1}} f(x)dx \approx \frac{h}{2}\left[f(x_k) + f(x_{k+1})\right]$$

- Then, adding up all the partial integrals we get:

$$\boxed{T(h) = \frac{h}{2}\left[f(x_0) + 2\left(f(x_1) + \cdots + f(x_{N-1})\right) + f(x_N)\right]}$$

Composite Trapezium

- Moreover, as the error produced in the computation of the integral in each subinterval is:

$$I_k(f) - T_k(h) = -\frac{f''(\xi_k)}{12} h^3, \qquad \xi_k \in \left(x_k, x_{k+1}\right)$$

- The total error will be:

$$I(f) - T(h) = -\frac{1}{12} h^3 \sum_{k=0}^{N-1} f''(\xi_k) = -\frac{h^2}{12} \frac{(b-a)}{N} \sum_{k=0}^{N-1} f''(\xi_k)$$

Composite Trapezium

- As we have that:

$$\min_{0\le k\le N} f''(\xi_k) \le \frac{1}{N}\sum_{k=0}^{N-1} f''(\xi_k) \le \max_{0\le k\le N} f''(\xi_k)$$

- There is some point ξ, within the interval defined by the values ($\min \xi_k$, $\max \xi_k$) for which

$$f''(\xi) = \frac{1}{N}\sum_{k=0}^{N-1} f''(\xi_k)$$

Composite Trapezium

- And finally, the total error is:

$$E(h) = I(f) - T(h) = -\frac{b-a}{12} h^2 f''(\xi)$$

- If $f''(x)$ is a continuous function in $[a, b]$, it is also bounded and increasing the number of divisions (with smaller h), we will increase our precision as h^2. The total error is then limited only by the machine precision.

Composite Simpson

- We can work out a similar composite quadrature formula using Simpson's Rule. In this case, however, we will have the ***additional restriction*** that the ***number of abscissas*** $N+1$ ***must be odd***, while the ***number of divisions*** N ***must be even***.
- We will divide the domain using consecutive intervals written as $[x_{2k}, x_{2k+1}]$, $k = 0,1,\ldots,N/2-1$ to use the composite Simpson's Rule

Composite Simpson

- The restriction of the integral in each of these intervals can be written as:

$$I_k(f) = \frac{h}{3}\left[f(x_{2k}) + 4f(x_{2k+1}) + f(x_{2k+2})\right]$$

- As the term $f(x_{2k+2})$ appears in the computation of I_k as well as in I_{k+1} we obtain:

$$\boxed{S(h) = \frac{h}{3}\left[f(x_0) + 4\sum_{k=0}^{N/2-1} f(x_{2k+1}) + 2\sum_{k=0}^{N/2-2} f(x_{2k+2}) + f(x_N)\right]}$$

Composite Simpson

- Proceeding as in the case of the Trapezium composite rule we can also evaluate the error term, resulting in:

$$I(f) - S(h) = -\frac{N/2}{90} h^5 f^{(4)}(\xi) = -\frac{b-a}{180} h^4 f^{(4)}(\xi)$$

- In the case of bounded continuous derivatives, the error will be of the order of h^4
- Note that the rule will be exact for polynomials of third degree.

Testing

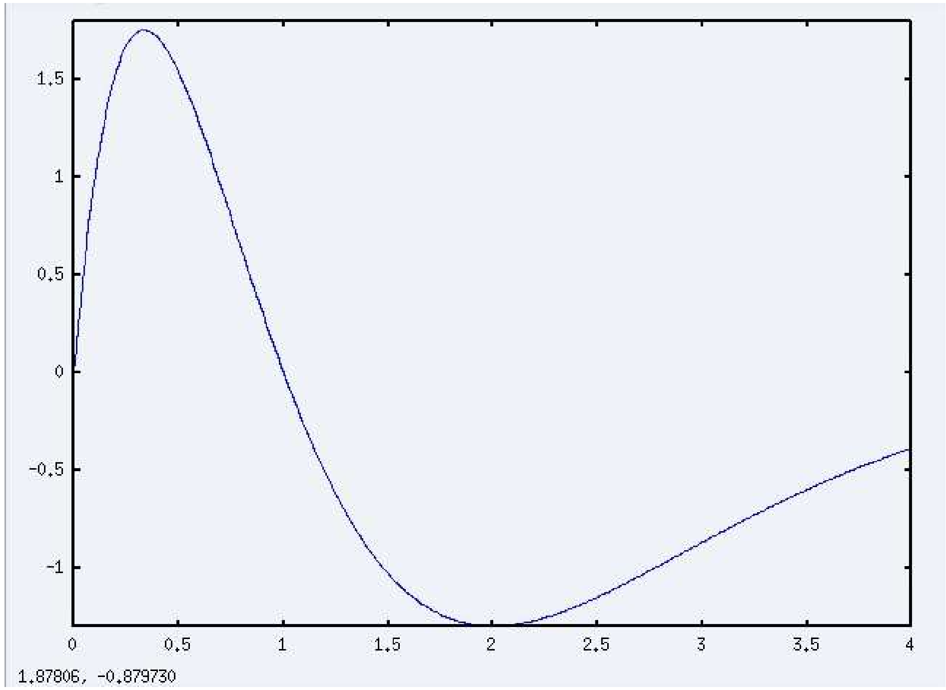
- We can compare the performance of these algorithms when they are applied to the computation of the following integral which can be computed exactly:

$$\int_0^4 13(x - x^2)e^{-3x/2}dx = \frac{4108e^{-6} - 52}{27}$$

$$= -1.5487883725279481333;$$

```
function ftest = ftest(x)
ftest = 13.0*(x-x*x)*exp(-3*x/2);
```

- Which can be represented graphically:



Testing

- It is easy to apply the composite trapezium and Simpson rules using 10, 100 and 1000 divisions of the interval [0,4]

test_t.m | test_s.m

```
%test trapecic
x=0:0.01:4;
for i=1:length(x)
  fp(i)=feval('ftest',x(i));
end
xlabel('x');
ylabel('y');
plot(x,fp);
format long
trapecic('ftest',0,4,10)
trapecic('ftest',0,4,100)
trapecic('ftest',0,4,1000)
```

test_s.m

```
%test trapecic
x=0:0.01:4;
for i=1:length(x)
  fp(i)=feval('ftest',x(i));
end
xlabel('x');
ylabel('y');
plot(x,fp);
format long
simpsonc('ftest',0,4,10)
simpsonc('ftest',0,4,100)
simpsonc('ftest',0,4,1000)
```

Testing

- The results obtained are:

```
octave:34> test_t
ans = -1.71027887162231
ans = -1.55047371674105
ans = -1.54880523317309
octave:36> test_s
ans = -1.57485038550214
ans = -1.54879128022895
ans = -1.54878837281904
```

- Which should be compared with the exact value

$$\int_0^4 13(x-x^2)e^{-3x/2}dx = -1.5487883725279481333;$$

Romberg Integration

- This algorithm allows to compute integrals with great precision. It is based in the fact that the composite quadrature formulas can be written as:

$$I(f) = \int_a^b f(x)dx = T(h) + E(h)$$

- Where $h = (b-a)/n$ and $E(h)$ represents the error term, which can be written as a power series. In the case of the composite Simpson rule:

$$E(h) = \frac{b-a}{180} h^4 f^{(4)}(\xi) = c_1 h^4 + c_2 h^8 + c_3 h^{12} + \cdots$$

Romberg Integration

- Romber integration may be formulated as follow. Let I be the exact value of the integral and T_i the approximate value of the integral obtained using Simpson's rule with i intervals. Then:

$$I = T_i + c_1 h^4 + c_2 h^8 + c_3 h^{12} + \cdots$$

- Doubling the number of intervals or halving h, we have

$$I = T_{2i} + c_1 \left(h/2\right)^4 + c_2 \left(h/2\right)^8 + c_3 \left(h/2\right)^{12} + \cdots$$

Romberg Integration

- We can eliminate the terms in h^4 by subtracting 16 times the second equation from the firs to obtain:

$$I = \frac{16T_{2i} - T_i}{15} + k_2 h^8 + k_3 h^{12} + \cdots$$

- The dominant term of the error is now of $O(h^8)$ increasing considerably the precision of the approximation. If we generate an initial set of approximations by successively halving the interval, we may use this idea further to obtain much better approximate values.

Romberg Integration

- If we represent these initial approximations by $T_{0,k}$, where the values $k = 0,1,2,\ldots$ represent the times we halve the intervals we can use the recursive formula

$$T_{r,k} = \frac{16^r T_{r-1,k-1} - T_{r-1,k}}{\left(16^r - 1\right)}, \quad k = 0,1,2,\ldots, \quad r = 1,2,3,\ldots$$

- To obtain the following set of approximations:

$$\begin{array}{lllll} T_{0,0} & T_{0,1} & T_{0,2} & T_{0,3} & \cdots \\ T_{1,0} & T_{1,1} & T_{1,2} & \vdots & \\ T_{2,0} & T_{2,1} & \vdots & & \\ T_{3,0} & \vdots & & & \\ \vdots & & & & \end{array}$$

Romberg Integration

- Halving the step *h*, we can obtain better approximations filling this table using the recurrence relation. The last term of the table will be the approximation of better precision.
- We can continue the halving of the intervals on and on:

$$\left(b-a\right)/2^{k} \quad \text{for} \quad k=0,1,2,\ldots$$

- Until we reach the precision of the machine if needed.

Adaptative Quadrature

- The composite quadrature formulas use evenly spaced nodes. If we want to reach a good precision, we will be forced, normally to use small step values, h.
- Using the composite formulas, we cannot take in account a situation where the integrating function can have rapid variation in some zones while in others may be nearly constant. All these zones will be divided with the same intensity.

Adaptative Quadrature

- It would be a clever procedure to use small steps only in the rapid variation zones.
- The adaptative method does exactly this. It is based on Simpson's Rule. Suppose that we want to integrate $f(x)$ in $[a_k, b_k]$. We write

$$S(a_k, b_k) = \frac{h}{3}\left(f(a_k) + 4f(c_k) + f(b_k)\right)$$

- Where $c_k = (a_k + b_k)/2$ and $h = (b_k - a_k)/2$.

Adaptative Quadrature

- If $f(x)$ is a smooth function and has derivatives of high order:

$$\int_{a_k}^{b_k} f(x)dx = S(a_k, b_k) - h^5 \frac{f^{(4)}(d_1)}{90}$$

- Where d_1 is in $[a_k, b_k]$. Using the composite rule with four intervals using half the step $(h/2)$ we have

$$S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) = \frac{h}{6}\big(f(a_{k1}) + 4f(c_{k1}) + f(b_{k1})\big)$$
$$+\frac{h}{6}\big(f(a_{k2}) + 4f(c_{k2}) + f(b_{k2})\big)$$

Adaptative Quadrature

- While the error in this case is:

$$\int_{a_k}^{b_k} f(x)dx = S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) - 2\left(\frac{h}{2}\right)^5 \frac{f^{(4)}(d_2)}{90}$$

$$= S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) - \frac{h^5}{16}\frac{f^{(4)}(d_2)}{90}$$

- Where d_2 is also in $[a_k, b_k]$. If this interval is small enough, we can assume that:

$$f^{(4)}(d_1) \approx f^{(4)}(d_2)$$

Adaptative Quadrature

- And then:

$$S(a_k,b_k) - h^5 \frac{f^{(4)}(d_1)}{90} \approx S(a_{k1},b_{k1}) + S(a_{k2},b_{k2}) - \frac{h}{16}^5 \frac{f^{(4)}(d_2)}{90}$$

- We can estimate the error in the second quadrature using the computed values:

$$-h^5 \frac{f^{(4)}(d_2)}{90} \approx \frac{16}{15}\left(S(a_{k1},b_{k1}) + S(a_{k2},b_{k2}) - S(a_k,b_k)\right)$$

Adaptative Quadrature

- This procedure allows to estimate the error with a new division of the interval:

$$\left| \int_{a_k}^{b_k} f(x)dx - S(a_{k1}, b_{k1}) - S(a_{k2}, b_{k2}) \right|$$

$$\approx \frac{1}{10} \left| S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) - S(a_k, b_k) \right|$$

- Where we will compensate the rough approximation of $f^{(4)}(d_1) \sim f^{(4)}(d_2)$ using the value $1/10$ instead of $1/15$.

Adaptative Quadrature

- We can use an iterative process to refine our quadrature in each interval. Thus, is we want to reach a certain precision ε_k and

$$\frac{1}{10}\left|S(a_{k1},b_{k1})+S(a_{k2},b_{k2})-S(a_k,b_k)\right|<\varepsilon_k$$

- We do not need to make a new division of the integral. Otherwise, we will continue to divide this section.

Adaptative Quadrature

- If we want to reach a precision such that:

$$\left| \int_{a_k}^{b_k} f(x)dx - S(a_{k1}, b_{k1}) - S(a_{k2}, b_{k2}) \right| < \varepsilon_k$$

- If this relation is not satisfied, we need to divide in two the interval and assign half the error to each subinterval.
- Note that this iterative procedure should stop somewhere as the precision is getting better at each step by the factor 1/16.

Adaptative Quadrature

- We can apply also this method to the former exact integral

$$\int_0^4 13(x - x^2)e^{-3x/2}dx = -1.5487883725279481333;$$

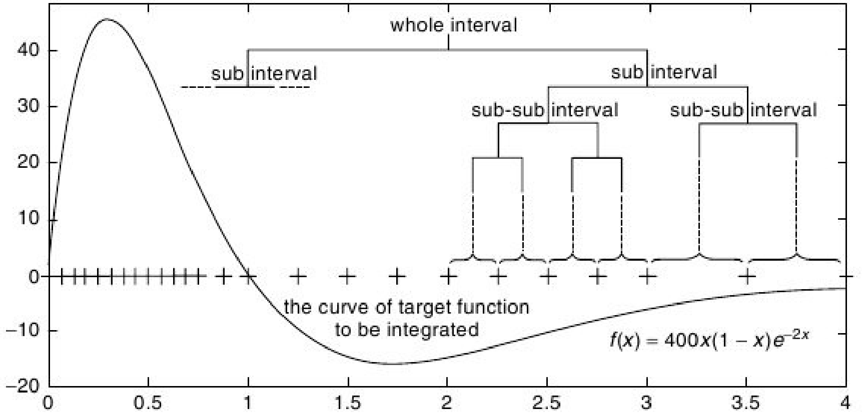


Figure 5.4 The subintervals (segments) and their boundary points (nodes) determined by the adaptive Simpson method.

Adaptative Test

test_a.m | srule.m | adapt.m

```
%test trapecic
x=0:0.01:4;
for i=1:length(x)
  fp(i)=feval('ftest',x(i));
end
xlabel('x');
ylabel('y');
plot(x,fp);
format long
[Srmat, quad, err]=adapt('ftest',0,4,0.001);
quad
err
[Srmat, quad, err]=adapt('ftest',0,4,0.0001);
quad
err
[Srmat, quad, err]=adapt('ftest',0,4,0.00001);
quad
err
```

```
octave:46> test_a
quad = -1.54898075337545
err =  4.06597665166236e-04
quad = -1.54877533794276
err =  3.46220348909791e-05
quad = -1.54878823412532
err =  2.96808615813113e-06
```

25279481333;

Gaussian Quadrature

- The formulas of Gaussian quadrature are based on the Legendre polynomials:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}\left[\left(x^2 - 1\right)^n\right], \qquad n = 0, 1, 2, \ldots$$

- The Legendre polynomial $P_n(x)$ will have n real roots in the interval $(-1,1)$ and verify the relations:

$$P_n(1) = 1$$

$$P_n(-1) = (-1)^n$$

Gaussian Quadrature

- Moreover, these polynomials satisfy the relations:

$$\int_{-1}^{1} P_n(x)Q_k(x)dx = 0, \quad k < n, \quad n = 0,1,2,\ldots$$

- The Legendre polynomial of degree n is orthogonal to all polynomials of lower degree.
- The Gaussian formulas of quadrature are developed in the interval $[-1,1]$ to make use of this property.

Gaussian Quadrature

- The objective is to obtain an expression of the form:

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

- Choosing the interpolating abscissas $t_1, t_2, \dots, t_n$ in such a way that the quadrature formula is exact for polynomials of the maximum degree as possible. As we have n abscissas and n free constants A_i, this degree should be $2n - 1$

Gaussian Quadrature

- Due to the orthogonality property, it will be sufficient to find a quadrature formula exact for the monomials $1, t, t^2, \dots, t^{2n-1}$. If we write:

$$\int_{-1}^{1} t^k dt = \sum_{i=1}^{n} A_i t_i^k, \qquad k = 0, 1, 2, \dots, 2n-1$$

- And write $f(t)$ as a linear combination of the monomials:

$$f(t) = \sum_{k=0}^{2n-1} C_k t^k$$

Gaussian Quadrature

- The following formula must be exact:

$$\int_{-1}^{1} f(t)dt = \sum_{k=0}^{2n-1} C_k \int_{-1}^{1} t^k dt = \sum_{k=0}^{2n-1} C_k \sum_{i=1}^{n} A_i t_i^k$$

$$= \sum_{i=1}^{n} A_i \sum_{k=0}^{2n-1} C_k t_i^k = \sum_{i=1}^{n} A_i f(t_i)$$

- Now, as we have:

$$\int_{-1}^{1} t^k dt = \frac{1-(-1)^{k+1}}{k+1} = \begin{cases} \dfrac{2}{k+1}, & \text{if } k \text{ odd} \\ 0 & \text{if } k \text{ even} \end{cases}$$

Gaussian Quadrature

- We can obtain the following set of equations when we apply this expression to the different monomials:

$$\left.\begin{aligned}
&\sum_{i=1}^{n} A_i = 2 \\
&\sum_{i=1}^{n} A_i t_i = 0 \\
&\vdots \\
&\sum_{i=1}^{n} A_i t_i^{2n-2} = \frac{2}{2n-1} \\
&\sum_{i=1}^{n} A_i t_i^{2n-1} = 0
\end{aligned}\right\}$$

Gaussian Quadrature

- However, this is a non-linear system, and it will be difficult to solve to obtain the coefficients A_i
- Consider then the polynomials:

$$Q_{n+k}(t) = t^k P_n(t), \qquad k = 0,1,\ldots,n-1$$

- Where $P_n(t)$ denotes the Legendre polynomial of degree n. Note that the polynomials built in this way, will never be of degree greater than $2n-1$.

Gaussian Quadrature

- Using the quadrature formula, we have:

$$\int_{-1}^{1} t^k P_n(t)dt = \sum_{i=1}^{n} A_i f(t_i) = \sum_{i=1}^{n} A_i t_i^k P_n(t_i), \qquad k = 0,1,\ldots,n-1$$

- However, the Legendre polynomial of degree n is orthogonal to the monomials t^k, and it must be true that:

$$\sum_{i=1}^{n} A_i t_i^k P_n(t_i) = 0, \qquad k = 0,1,\ldots,n-1$$

Gaussian Quadrature

- These equations can be satisfied if we use as the nodes t_i, the n zeros of the Legendre polynomial $P_n(t)$ within the interval $(-1,1)$ as we have:

$$P_n(t_i) = 0, \qquad i = 1, 2, \ldots, n$$

- All these zeros are real and distinct. We can then use the first n equations of the main system to obtain the values of the constants A_i. This linear system will have always a single solution as its determinant is the Vandermonde determinant:

$$D = \prod_{i>j} (t_i - t_j) \neq 0$$

- Consider for example the Gaussian quadrature formula for 3 abscissas. The Legendre polynomial of third degree is:

$$P_3(t) = \frac{1}{2}\left(5t^3 - 3t\right)$$

- The zeros of this polynomial are located at the values:

$$t_1 = -\sqrt{\frac{3}{5}}, \qquad t_2 = 0, \qquad t_3 = \sqrt{\frac{3}{5}}$$

Gaussian Quadrature

- Using these values we obtain the system of equations:

$$\begin{cases} A_1 + A_2 + A_3 = 2 \\ -\sqrt{\dfrac{3}{5}}A_1 + \sqrt{\dfrac{3}{5}}A_3 = 0 \\ \dfrac{3}{5}A_1 + \dfrac{3}{5}A_3 = \dfrac{2}{3} \end{cases} \Rightarrow \quad A_1 = A_3 = \frac{5}{9}, \qquad A_2 = \frac{8}{9}$$

- Which gives the formula

$$\int_{-1}^{1} f(t)dt = \frac{1}{9}\left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right)\right]$$

Gaussian Quadrature

- These formulas can be extended to any interval. If we want to compute the integral:

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

- We will need the linear transformation:

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

Gaussian Quadrature

- Then:

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

- And the quadrature formula becomes:

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

- With

$$x_i = \frac{b+a}{2}+\frac{b-a}{2}t_i, \quad i=1,2,\ldots,n$$