**Chapter 5  Numerical integration**

**Problem:** Let \( f : [a, b] \subset \mathbb{R} \rightarrow \mathbb{R} \) be a piecewise continuous function.

Compute the integral

\[
I(f) = \int_a^b f(x) \, dx.
\]

If \( I(f) \) can not be determined in closed form, we have to use a numerical method which is known as **numerical quadrature** resp. **numerical integration**.

**5.1 Newton-Cotes formulas**

**Example 5.1  Trapezoidal sum**

**Idea:** Partition of the domain of integration \([a, b]\) into \( n \) subintervals \( a = x_0 < x_1 < \ldots < x_n = b \) of length \( h_i := x_{i+1} - x_i \) and approximation of \( I(f) \) by the **sum of the trapezoids**

\[
T^{(n)} = \sum_{i=0}^{n-1} T_i, \quad T_i = \frac{h_i}{2} [f(x_i) + f(x_{i+1})] \quad \Rightarrow \\
\hat{I}(f) = \sum_{i=0}^{n} \lambda_i f(x_i), \quad \lambda_0 = \frac{h_0}{2}, \quad \lambda_i = \frac{(h_{i-1} + h_i)}{2}, \quad \lambda_n = \frac{h_{n-1}}{2}.
\]
Definition 5.2 Quadrature formula
A finite sum of weighted function values of the form
\[ \hat{I}(f) := \sum_{i=0}^{n} \lambda_i f(x_i) \]
for the approximation of \( I(f) = \int_{a}^{b} f(x) \, dx \) is called a quadrature formula. The points \( x_i, 0 \leq i \leq n \), are referred to as the nodes and the numbers \( \lambda_i, 0 \leq i \leq n \), are called the weights of the quadrature formula.

Remark 6.3 Quadrature formulas based on interpolation
In the special case \( n = 1 \), the trapezoidal sum reduces to the trapezoidal rule
\[ \hat{I}(f) = \frac{b-a}{2} [f(a) + f(b)] , \]
which can be obtained formally by replacing the integrand by its linear interpolant
\[ \hat{f} := p_1(f) = \frac{x-a}{b-a} [f(b) - f(a)] + f(a) \implies \hat{I}(f) = I(\hat{f}) = \int_{a}^{b} \hat{f}(x) \, dx . \]
Idea: Replacement of the integrand by its polynomial interpolant with respect to \((x_i, f(x_i)), \ 0 \leq i \leq n:\)

\[
\hat{f}(x) = p_n(f) = \sum_{i=0}^{n} f(x_i) L_{i,n}(x),
\]

where \(L_{i,n}(\cdot), 0 \leq i \leq n,\) denote the Lagrangian fundamental polynomials.

**Definition 5.4 Newton-Cotes formulas**

The quadrature formulas given by

\[
\hat{I}(f) = (b - a) \sum_{i=0}^{n} \alpha_{in} f(x_i), \quad \alpha_{in} := \frac{1}{b - a} \int_{a}^{b} L_{i,n}(x) \, dx, \ 0 \leq i \leq n
\]

are called Newton-Cotes formulas. The weights \(\alpha_{in}, 0 \leq i \leq n,\) are dubbed Newton-Cotes weights. The error \(I(f) - \hat{I}(f)\) is referred to as quadrature error.
Remark 5.5 Computation of the Newton-Cotes weights

In case of equidistant partitions of mesh width \( h := (b - a)/n \), the substitution \( t := (x - a)/h = n (x - a)/(b - a) \) yields:

\[
\alpha_{in} = \frac{1}{b-a} \int_a^b \frac{x-x_j}{\prod_{j \neq i} x_i - x_j} \, dx = \frac{1}{n} \int_0^n \frac{t-j}{\prod_{j \neq i} i-j} \, dt,
\]

and hence:

\[
\sum_{i=0}^{n} \alpha_{in} = 1 , \quad \alpha_{n-i,n} = \alpha_{i,n} , \quad 0 \leq i \leq n .
\]

The following table contains the Newton-Cotes formulas for \( n = 1, 2, 3, 4 \):

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \alpha_{in} )</th>
<th>error</th>
<th>name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(\frac{1}{2} )</td>
<td>(h^3/12 f^{(2)}(\xi))</td>
<td>trapezoidal rule</td>
</tr>
<tr>
<td>2</td>
<td>(\frac{1}{6} )</td>
<td>(h^5/90 f^{(4)}(\xi))</td>
<td>Simpson’s rule</td>
</tr>
<tr>
<td>3</td>
<td>(\frac{1}{8} )</td>
<td>(3h^5/80 f^{(4)}(\xi))</td>
<td>Kepler’s rule</td>
</tr>
<tr>
<td>4</td>
<td>(\frac{7}{90} )</td>
<td>(8h^7/945 f^{(6)}(\xi))</td>
<td>Milne’s rule</td>
</tr>
</tbody>
</table>

Observe that for \( n > 6 \) negative weights occur (cancellation!).
5.2 Gaussian quadrature

Problem: Given a natural number $n \in \mathbb{N}$, determine $n + 1$ nodes $x_{0n}, \ldots, x_{nn} \in [a, b]$ and $n + 1$ weights $\lambda_{0n}, \ldots, \lambda_{nn}$ such that for a weight function $\omega : (a, b) \rightarrow \mathbb{R}, \omega(x) < 0$, $x \in (a, b)$, the weighted integral

$$I(f) = \int_{a}^{b} \omega(x) f(x) \, dx$$

is integrated by the quadrature formula

$$\hat{I}(f) = \sum_{i=0}^{n} \lambda_{in} f(x_{in})$$

exactly for polynomials $p_{N} \in P_{N}([a, b])$ up to a maximal order $N$:

$$\hat{I}(p_{N}) = I(p_{N}) \quad , \quad p_{N} \in P_{N}([a, b]).$$

Number of free parameters: $2n + 2$.

Consequence: Polynomials $p_{N} \in P_{N}([a, b])$, $N \leq 2n + 1$ will be integrated exactly.
Theorem 5.6 Gaussian quadrature formulas

Let \( p_0, ..., p_{n+1} \) be the orthogonal polynomials with respect to the inner products

\[
(f, g) = \int_a^b \omega(x) f(x) g(x) \, dx
\]

with leading coefficient 1. Denote by \( x_{0n}, ..., x_{nn} \) the \( n+1 \) simple zeroes of \( p_{n+1} \) in \((a, b)\). Then, for the weights

\[
\lambda_{in} = \int_a^b \omega(x) \frac{p_{n+1}(x)}{(x - x_{in}) p'_{n+1}(x_{in})} \, dx, \quad 0 \leq i \leq n
\]

there holds:

\[
\hat{I}(p) = I(p), \quad p \in P_{2n+1}([a, b]) .
\]

**Proof:** Let \( p \in P_{2n+1}([a, b]) \). Then, there exist \( q, r \in P_n([a, b]) \) such that

\[
p = q \, p_{n+1} + r ,
\]

and hence,

\[
p(x_{in}) = q(x_{in}) \, p_{n+1}(x_{in}) + r(x_{in}) = r(x_{in}), \quad 0 \leq i \leq n .
\]
Further, let
\[ r = \sum_{i=0}^{n} r(x_i) L_{in} = \sum_{i=0}^{n} p(x_i) L_{in} \]
be the representation of \( r \) as the Lagrangian interpolating polynomial with respect to the nodes \( x_{0n}, ..., x_{nn} \). Then, there holds:
\[
I(p) = \int_{a}^{b} \omega(x) p(x) \, dx = \int_{a}^{b} \omega(x) q(x) p_{n+1}(x) \, dx + \int_{a}^{b} \omega(x) r(x) \, dx = 0
\]
\[
= \sum_{i=0}^{n} p(x_i) \int_{a}^{b} \omega(x) L_{in}(x) \, dx .
\]
Moreover, we have
\[
L_{in}(x) = \prod_{k \neq i} \frac{x - x_{kn}}{x_i - x_{kn}} = \frac{p_{n+1}(x)}{\prod_{k \neq i} \frac{1}{x - x_i} x_{in} - x_{kn}} ,
\]
\[
p'_{n+1}(x) = \left[ \prod_{k=0}^{n} (x - x_{kn}) \right]' = \sum_{j=0}^{n} \prod_{k \neq j} (x - x_{kn}) \implies p'_{n+1}(x_{in}) = \prod_{k \neq i} (x_{in} - x_{kn}) ,
\]
whence
\[
L_{in}(x) = \frac{p_{n+1}(x)}{(x - x_{in}) p'_{n+1}(x_{in})} .
\]
Remark 5.7 Properties of the weights
Taking advantage of the properties of orthogonal polynomials, it can be shown that all weights of Gaussian quadrature formulas are positive, i.e. $\lambda_{in} > 0$, $0 \leq i \leq n$.

The following table provides a listing of specific weight functions, associated intervals, and orthogonal polynomials:

<table>
<thead>
<tr>
<th>Name of quadrature formula</th>
<th>$[a, b]$</th>
<th>$\omega(\alpha, \beta)$</th>
<th>$p_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gauss-Legendre</td>
<td>$[-1, +1]$</td>
<td>1</td>
<td>$P_n$</td>
</tr>
<tr>
<td>Gauss-Chebyshev</td>
<td>$[-1, +1]$</td>
<td>$(1 - x^2)^{-1/2}$</td>
<td>$T_n$</td>
</tr>
<tr>
<td>Gauss-Jacobi</td>
<td>$[-1, +1]$</td>
<td>$(1 - x)^\alpha(1 + x)\beta$</td>
<td>$P_n^{(\alpha, \beta)}$</td>
</tr>
<tr>
<td>Gauss-Laguerre</td>
<td>$[0, \infty)$</td>
<td>$x^\alpha \exp(-x)$</td>
<td>$L_n^{(\alpha)}$</td>
</tr>
<tr>
<td>Gauss-Hermite</td>
<td>$(-\infty, +\infty)$</td>
<td>$\exp(-x^2)$</td>
<td>$H_n$</td>
</tr>
</tbody>
</table>
Theorem 5.8  Approximation error  
Let \( f \in C^{2n+2}([a, b]) \), where \(-\infty \leq a < b \leq +\infty\), and assume that \( \max_{x \in [a, b]} |f^{(k)}(x)| < \infty \), \( 0 \leq k \leq 2n + 2 \).

Then, there holds
\[
| \hat{I}(f) - I(f) | \leq (p_{n+1}, p_{n+1}) \max_{x \in [a, b]} |f^{(2n+2)}(x)| \left( \frac{1}{(2n + 2)!} \right).
\]

Proof: Let \( \hat{f} \in P_{2n+1}([a, b]) \) be the Hermitian interpolating polynomial with respect to \( x_i, 0 \leq i \leq n \):
\[
\hat{f}(x_i) = f(x_i), \quad \hat{f}'(x_i) = f'(x_i), \quad 0 \leq i \leq n.
\]
\( \hat{f} \) has the representation:
\[
\hat{f}(x) = \sum_{i=0}^{n} (c_{in} x + d_{in}) \mathcal{L}_{in}^2(x) f(x_{in}) + \sum_{i=0}^{n} (x - x_{in}) \mathcal{L}_{in}^2(x) f'(x_{in}),
\]
with \( c_{in} := -2 \prod_{j \neq i} \frac{1}{x_{in} - x_{jn}} \), \( d_{in} := 1 - c_{in} x_{in} \), \( 0 \leq i \leq n \).
According to the representation of the remainder for Hermitian interpolation, we have:

\[ f(x) - \hat{f}(x) = \frac{f(2n+2)(\xi(x))}{(2n+2)!} \prod_{i=0}^{n} (x - x_{in})^2 = \frac{f(2n+2)(\xi(x))}{(2n+2)!} p_{n+1}^2(x), \]

where \( \xi(x) \in (\min_{0 \leq i \leq n} (x, x_{in}), \max_{0 \leq i \leq n} (x, x_{in})) \). The mean value theorem of calculus implies that for an appropriate \( \xi \in (a, b) \):

\[ I(f - \hat{f}) = \frac{f(2n+2)(\xi)}{(2n+2)!} \int_{a}^{b} \omega(x) p_{n+1}^2(x) \, dx = \frac{f(2n+2)(\xi)}{(2n+2)!} (p_{n+1}, p_{n+1}). \]

On the other hand, observing \( \hat{f} \in P_{2n+1}([a, b]) \):

\[ I(\hat{f}) = \int_{a}^{b} \omega(x) \hat{f}(x) \, dx = \sum_{i=0}^{n} \lambda_{in} \hat{f}(x_{in}) = \sum_{i=0}^{n} \lambda_{in} f(x_{in}) = \hat{I}(f), \]

which proves the assertion.
5.3 Romberg integration

The trapezoidal sum admits an asymptotic expansion in $h^2$ of the steplength $h = (b - a)/n$.

Idea: Computation of the trapezoidal sum for different steplengths and suitable combination of the results to obtain a higher order approximation $\implies$ extrapolation method

5.3.1 Asymptotic expansion of the trapezoidal sum

We consider the trapezoidal sum

$$\displaystyle T(h) = h \left[ \frac{1}{2} f(a) + \sum_{i=1}^{n-1} f(a + ih) + \frac{1}{2} f(b) \right]$$

with respect to equidistant nodes $x_i = a + ih$, $0 \leq i \leq n$, $h := (b - a)/n$, $n \in \mathbb{N}$.

Theorem 5.9 Euler-MacLaurin summation formula

Assume $f \in C^{2m+2}([a, b])$, $m \in \mathbb{N}$. Then, the trapezoidal sum $T(h)$ has the asymptotic expansion

$$\displaystyle T(h) = \int_{a}^{b} f(x) \, dx + \sum_{k=1}^{m} \tau_{2k} h^{2k} + R_{2m+2}(h) h^{2m+2}.$$
The coefficients $\tau_{2k}$, $1 \leq k \leq m$, are given by

$$\tau_{2k} = \frac{(-1)^{k+1} B_k}{(2k)!} \left[ f'(2k-1)(b) - f'(2k-1)(a) \right],$$

where $B_k$, $1 \leq k \leq m$, are the Bernoulli numbers $B_k := (-1)^{k+1}B_{2k}(0)$ with $B_k(\cdot)$ denoting the Bernoulli polynomials which are recursively given according to

$$B_0(x) = 1, \quad B'_k(x) = k B_{k-1}(x), \quad k \geq 1$$

The remainder term admits the representation

$$R_{2m+2}(h) = - \int_a^b K_{2m+2}(x; h) f^{(2m+2)}(x) \, dx$$

and is uniformly bounded in $h$, i.e., there exists a constant $C_{2m+2} \geq 0$, independent of $h$ such that for all $h = (b - a)/n$:

$$|R_{2m+2}(h)| \leq C_{2m+2} |b - a|.$$
5.3.2 Extrapolation methods

Idea behind extrapolation: If \( f \in C^4([a,b]) \) and if the trapezoidal sum \( T(\cdot) \) is computed with respect to the steplengths \( h \) and \( h/2 \), in view of Theorem 5.9 we have:

\[
(+) \quad T(h) = \int_a^b f(x) \, dx + \tau_2 h^2 + O(h^4),
\]

\[
(++) \quad T(h/2) = \int_a^b f(x) \, dx + \frac{1}{4} \tau_2 h^2 + O(h^4).
\]

Multiplication of \((++)\) by 4 and subtraction of \((+)\) yields an approximation of order \( O(h^4)\):

\[
\frac{4}{3} T(h/2) - \frac{1}{3} T(h) = \int_a^b f(x) \, dx + O(h^4).
\]

We have:

\[
\frac{4}{3} T(h/2) - \frac{1}{3} T(h) = T(h) + \frac{4}{3} \left[ T(h/2) - T(h) \right].
\]
There holds:

$$\left(\star\right) \frac{4 T(h/2) - T(h)}{3} = T(h) + \frac{4}{3} \left[ T(h/2) - T(h) \right].$$

On the other hand, the interpolating polynomial in $t^2$ associated with the pairs $(h^2, T(h))$ and $(h^2/4, T(h/2))$ is given by

$$p(T(t) \mid h^2, \frac{1}{4} h^2)(t^2) = T(h) - \frac{4}{3} \frac{T(h/2) - T(h)}{h^2} (t^2 - h^2).$$

We realize that $\left(\star\right)$ corresponds to the value of the interpolating polynomial in $t^2 = 0$. Therefore, this technique is referred to as **extrapolation to the steplength** $h = 0$.

A generalization of this idea allows for approximations of arbitrary order, provided the function $f$ is sufficiently smooth.

We consider the following scenario:

Let $H := \{ h_n \in \mathbb{R}_+ \ , \ n \in \mathbb{N} \ , \ h_n \to 0 \ (n \to \infty) \}$ be a null sequence of positive real numbers and $T(h), h \in H$, a method for the computation of a value $\tau_0 \in \mathbb{R}$ such that

$$\lim_{h \to 0} T(h) = \tau_0.$$
Definition 5.10  Asymptotic expansion

The method $T(h)$ for the computation of $\tau_0$ is said to have an asymptotic expansion in $h^p$, $p \in \mathbb{N}$, up to the order $pm$, $m \in \mathbb{N}$, if there exist constants $\tau_{kp}$, $1 \leq k \leq m$, such that

$$T(h) = \tau_0 + \sum_{k=1}^{m} \tau_{kp} h^p + O(h^{(m+1)p}) \ (h \to 0).$$

We compute $T(h)$ for $k$ steplengths $h = h_{i-k+1}, \ldots, h_i$ and determine the interpolating polynomial in $h^p$:

$$p_{ik}(h^p) = p(h^p | h_{i-k+1}^p, \ldots, h_i^p) \text{ in } P_{k-1}(h^p)$$

associated with the pairs $(h_j^p, T(h_j))$, $i - k + 1 \leq j \leq i$. We denote by $T_{ik}$ the extrapolated value at $h = 0$, i.e.,

$$T_{ik} = p_{ik}(0) \quad , \quad 1 \leq k \leq i.$$
According to the algorithm of Aitken-Neville, the values $T_{ik}$ can be computed recursively as follows:

$$T_{i1} := T(h_i) , \quad i = 1, 2, \ldots ,$$

$$T_{ik} = T_{i,k-1} + \frac{T_{i,k-1} - T_{i-1,k-1}}{(h_{i+k-1}/h_i)p - 1} , \quad 2 \leq k \leq i .$$

We thus obtain the extrapolation table:

$$
\begin{array}{cccc}
T_{11} & & & \\
T_{21} & T_{22} & & \\
& & \ddots & \\
& & & \ddots \\
T_{k-1,1} & \cdots & \cdots & T_{k-1,k-1} \\
T_{k,1} & \cdots & \cdots & T_{k,k-1} & T_{k,k} \\
\end{array}
$$
Denoting the approximation error with respect to $T_{ik}$ by

$$\varepsilon_{ik} := -\tau_0 \mid , \; 1 \leq k \leq i ,$$

the following result shows that we theoretically gain the order $p$ per column of the extrapolation table:

**Theorem 5.11** Bulirsch’ theorem

Let $T(h)$ be a method for the computation of $\tau_0 \in \mathbb{R}$ which admits an asymptotic expansion in $h^p$ up to the order $pm$. Moreover, let $T_{ik} , \; 1 \leq k \leq i \leq m$, be the approximations computed by extrapolation to the steplength $h = 0$ with respect to the steplengths $h_j , \; 1 \leq j \leq m$. Then, for the extrapolation error there holds

$$\varepsilon_{ik} = \mid \tau_{kp} \mid \prod_{j=i-k+1}^{i} h_j^p + \sum_{j=i-k+1}^{i} O(h_j^{(k+1)p}) , \; (h_j \leq h \to 0).$$
**Proof:** By assumption, for $1 \leq k \leq m$ there holds:

\[(•) \quad T_{j1} = T(h_j) = \tau_0 + \sum_{\ell=1}^{k} \tau_{\ell p} h_j^{\ell p} + O(h_j^{(k+1)p}) . \]

Now, let $p_{kk}(h^p) = p(h^p | h_1^p, ..., h_k^p)$ be the interpolating polynomial in $h^p$ with respect to $(h_j^p, T_{j1}), \ 1 \leq j \leq k$, which has the Lagrangian representation

$$p_{kk}(h^p) = \sum_{j=1}^{k} L_j(h^p) \ T_{j1} ,$$

where $L_j(h^p), \ 1 \leq j \leq k$, are the Lagrangian fundamental polynomials.

Using the identity

$$\sum_{j=1}^{k} L_j(0) \ h_j^{\ell p} = \begin{cases} 1 & , \ell = 0 \\ 0 & , 1 \leq \ell \leq k - 1 \\ (-1)^{k-1} \prod_{\nu=1}^{k} h_{\nu}^p & , \ell = k \end{cases}$$

and observing $(•)$, it follows that

$$T_{kk} = p_{kk}(0) = \sum_{j=1}^{k} L_j(0) \ T_{j1} = \sum_{j=1}^{k} L_j(0) [ \tau_0 + \sum_{\ell=1}^{k} \tau_{\ell p} h_j^{\ell p} + O(h_j^{(k+1)p}) ] =$$

$$= \tau_0 + (-1)^{k-1} \tau_{kp} \prod_{\nu=1}^{k} h_{\nu}^p + O(h_j^{(k+1)p}) ,$$

which gives the assertion for $i = k$. The cases $1 \leq k < i$ are shown analogously.
5.3.3 Implementation of the Romberg integration

The application of the previously described extrapolation technique to the numerical com-
putation of integrals is called Romberg integration resp. Romberg quadrature. We proceed in such a way that, given the basic steplenth $H > 0$, the steplengths $h_i, i \in \mathbb{N}$, are determined according to

$$h_i := \frac{H}{n_i}, \quad n_i \in \mathbb{N}, \ i = 0, 1, 2, \ldots .$$

Once $n_i, i = 0, 1, 2, \ldots$ has been specified, the method is characterized by the sequence of step-
lengths

$$\mathcal{F} = \{n_0, n_1, \ldots\} .$$

The selection of the steplengths depends on the computational work for the computation of the approximations $T_{ii}$ which is measured by the number $A_i$ of function evaluations. Hence, associated with the sequence of steplengths $\mathcal{F}$ there is the sequence of computational work

$$\mathcal{A} = \{A_0, A_1, \ldots\} .$$
In the following, we consider the so-called Romberg sequence as well as the Bulirsch sequence:

(i) Romberg sequence

The Romberg sequence follows by successively halving the basic steplength:

$$\mathcal{R} = \{2^i\}_{i \in \mathbb{N}_0} = \{1, 2, 4, 8, 16, \ldots\}.$$

If we observe

$$T(h/2) = \frac{h}{4} \left[ f(a) + 2 \sum_{i=1}^{2n-1} f(a + ih/2) + f(b) \right] =$$

$$= \frac{h}{4} \left[ f(a) + 2 \sum_{k=1}^{n-1} f(a + kh) + f(b) \right] + \frac{h}{2} \sum_{k=1}^{n} f\left(a + \frac{2k-1}{2} h\right) =$$

$$= \frac{1}{2} T(h) + \frac{h}{2} \sum_{k=1}^{n} f\left(a + \frac{2k-1}{2} h\right),$$

the trapezoidal sums can be computed recursively (note that $h_i = H/2^i$):

$$T_{i0} = \frac{1}{2} T_{i-1,0} + h_i \sum_{k=1}^{n_i-1} f\left(a + (2k - 1) h_i\right).$$

Consequently, for the sequence of computational work we obtain:

$$\mathcal{A}_R = \{n_i + 1\}_{i \in \mathbb{N}_0} = \{2, 3, 5, 9, 17, \ldots\}.$$
(ii) Bulirsch sequence
The Bulirsch sequence is a more advantageous sequence from the point of view of computational work:

\[ n_i = \begin{cases} 
2^k, & i = 2k - 1, \\
3 \cdot 2^{k-1}, & i = 2k, \\
1, & i = 0 
\end{cases} \]

whence

\[ \mathcal{F}_B = \{1, 2, 3, 4, 6, 8, 12, 16, 24, \ldots \} . \]

The associated sequence of computational work is given by:

\[ \mathcal{A}_B = \{2, 3, 7, 9, 13, 17, \ldots \} . \]

Computation of the extrapolation table:
The extrapolation table will be constructed row by row. It will be terminated, if
- some prespecified accuracy has been achieved or
- no improvement of the convergence occurs.
5.4 Adaptive multigrid quadrature

Example 5.12: Consider the function
\[ \int_{-1}^{1} \frac{1}{10^{-4} + x^2} \, dx \]

Idea: Start from a coarse partition \( \Delta^0 \) of the interval \([a, b]\) and successively generate finer partitions \( \Delta^1 \) by locally refining the partitions only there where required to achieve the prescribed accuracy.

Tools:
- Local estimator of the discretization error,
- Local refinement rules.
5.4.1 Local error estimator and refinement strategy

We choose the trapezoidal sum as the underlying method for the multigrid quadrature. We consider a partition $\Delta$ of $[a, b]$ with subintervals $J = [x_\ell, x_r] \subset [a, b]$:

$$T(\Delta) = \sum_{J \in \Delta} T(J).$$

The integral is decomposed analogously

$$\int_a^b f(x) \, dx = \sum_{J \in \Delta} \int_J f(x) \, dx.$$

Firstly, we are interested in an estimate of the local discretization error

$$| \int_{x_\ell}^{x_r} f(x) \, dx - T(J) |.$$

We know that the Simpson rule

$$S(J) = \frac{h}{6} \left[ f(x_\ell) + 4 f(x_m) + f(x_r) \right],$$

where $x_m := (x_\ell + x_r)/2$, is of an order higher than that of the trapezoidal rule and use it for comparison.
Under the assumption

\[(S) \quad | S(J) - \int_{x_l}^{x_r} f(x) \, dx | \leq q_J | T(J) - \int_{x_l}^{x_r} f(x) \, dx | , \quad 0 \leq q_J < 1 \]

there holds:

\[(\diamond) \quad \frac{1}{1 + q_J} | T(J) - S(J) | \leq | \int_{x_l}^{x_r} f(x) \, dx - T(J) | \leq \frac{1}{1 - q_J} | T(J) - S(J) | ,\]

i.e., the quantity

\[(\star) \quad \bar{\varepsilon}(J) := | T(J) - S(J) | \]

provides an upper and a lower bound for the local discretization error.

As a refinement rule, we choose the local bisection of an interval:
We thus obtain a binary tree characterizing the refinement process. We refer to $J_{\ell}$ as the father of $J_{\ell\ell}$ and $J_{\ell r}$ as well as the son of $J$. In the following, we denote the father of an interval $J$ by $J^-$. 

The principle for refinement of a partition $\Delta$ is based on the equidistribution of the local discretization error:

We refine the grid $\Delta$ such that for the local estimators with respect to the refined grid $\Delta^+$ there holds:

$$\bar{\varepsilon}(J) \approx \text{const.} \quad \text{for all } J \in \Delta^+. $$

Therefore, we are interested in another error estimator $\varepsilon^+(J)$ which provides information about the error $\varepsilon(J_{\ell})$ of the next level in case $J$ has been partitioned into $J_{\ell}$ and $J_r$. 
As far as the estimator $\bar{\varepsilon}(J)$ is concerned, we assume

$$\bar{\varepsilon}(J) \doteq C \, h^{\gamma} \quad (h = h(J)),$$

where $C > 0$ is a local constant and $\gamma > 1$. Then, it follows that

$$\bar{\varepsilon}(J^{-}) \doteq C \, (2h)^{\gamma} = 2^{\gamma} \, C \, h^{\gamma} \doteq 2^{\gamma} \, \bar{\varepsilon}(J) \quad \rightarrow \quad 2^{\gamma} \doteq \bar{\varepsilon}(J^{-})/\bar{\varepsilon}(J).$$

We thus obtain:

$$\varepsilon(J_{\ell}) \doteq C \left(\frac{h}{2}\right)^{\gamma} = 2^{-\gamma} \, C \, h^{\gamma} \doteq 2^{-\gamma} \, \bar{\varepsilon}(J) \doteq \bar{\varepsilon}(J)^{2}/\bar{\varepsilon}(J^{-}).$$

Consequently, the quantity

$$\varepsilon^{+}(J) :\doteq \frac{\bar{\varepsilon}(J)^{2}}{\bar{\varepsilon}(J^{-})}$$

may serve as the required error estimator.
The error estimator

$$\varepsilon^+(J) := \frac{\overline{\varepsilon}(J)^2}{\overline{\varepsilon}(J^-)}$$

can be interpreted in the local extrapolation.

We define:

$$\kappa(\Delta) := \max_{J \in \Delta} \varepsilon^+(J)$$

as the maximum local error in case of uniform refinement of $\Delta$. Then, it is appropriate to choose the following refinement rule: Refine $J \in \Delta$, if

$$\overline{\varepsilon}(J) \geq \kappa(\Delta).$$