# Chapter 5 Numerical integration

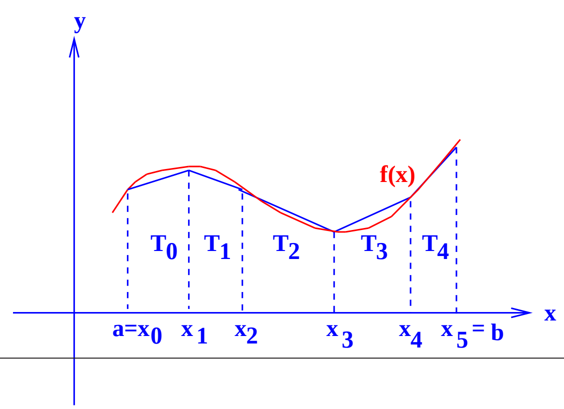
**Problem:** Let $f : [a,b] \subset \mathbb{R} \to \mathbb{R}$ be a piecewise continuous function.
Compute the integral

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

If $I(f)$ can not be determined in closed form, we have to use a numerical method which is 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 $a = x_0 < x_1 < ... < x_n = b$ of length $h_i := x_{i+1} - x_i$ and approximation of $I(f)$ by the sum of the trapezoids

$$T^{(n)} \ = \ \sum_{i=0}^{n-1} T_i \quad , \quad T_i \ = \ \frac{h_i}{2}\, [f(x_i) \ + \ f(x_{i+1})] \quad \Longrightarrow$$

$$\hat{I}(f) \ = \ \sum_{i=0}^{n} \lambda_i\, f(x_i) \quad , \quad \lambda_0 = \frac{h_0}{2} \ , \ \lambda_i = \frac{(h_{i-1}+h_i)}{2} \ , \ \lambda_n = \frac{h_{n-1}}{2} \ .$$

**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 $x_i, 0 \le i \le n,$ are referred to as the nodes and the numbers $\lambda_i, 0 \le i \le n,$ 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

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

which can be obtained formally by replacing the integrand by its linear interpolant

$$\hat{f} := p_1(f) = \frac{x-a}{b-a}\left[f(b) - f(a)\right] + f(a) \quad \Longrightarrow \quad \hat{I}(f) = I(\hat{f}) = \int_a^b \hat{f}(x)\, dx .$$

Idea: Replacement of the integrand by its polynomial interpolant with respect to $(x_i, f(x_i))$, $0 \le i \le n$:

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

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

**Definition 5.4 Newton-Cotes formulas**
The quadrature formulas given by

$$\hat{I}(f) \; = \; (b \; - \; a) \sum_{i=0}^{n} \alpha_{in}\, f(x_i) \quad , \quad \alpha_{in} \; := \; \frac{1}{b-a} \int_a^b L_{i,n}(x)\, dx \; , \; 0 \le i \le n$$

are called Newton-Cotes formulas. The weights $\alpha_{in}, 0 \le i \le n$, are dubbed Newton-Cotes weights. The error $I(f) - I(\hat{f})$ 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:

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

and hence:

$$\sum_{i=0}^{n}\alpha_{in} \;=\; 1 \quad , \quad \alpha_{n-i,n} \;=\; \alpha_{i,n}\,,\; 0\le i\le n\,.$$

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

| $n$ | $\alpha_{in}$ | | | | | error | name |
|---|---|---|---|---|---|---|---|
| 1 | $\frac{1}{2}$ | $\frac{1}{2}$ | | | | $h^3/12\, f^{(2)}(\xi)$ | trapezoidal rule |
| 2 | $\frac{1}{6}$ | $\frac{2}{3}$ | $\frac{1}{6}$ | | | $h^5/90\, f^{(4)}(\xi)$ | Simpson's rule |
| 3 | $\frac{1}{8}$ | $\frac{3}{8}$ | $\frac{3}{8}$ | $\frac{1}{8}$ | | $3h^5/80\, f^{(4)}(\xi)$ | Kepler's rule |
| 4 | $\frac{7}{90}$ | $\frac{16}{45}$ | $\frac{2}{15}$ | $\frac{16}{45}$ | $\frac{7}{90}$ | $8h^7/945\, f^{(6)}(\xi)$ | Milne's rule |

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 $x_{0n}, ..., x_{nn} \in [a,b]$ and $n+1$ weights $\lambda_{0n}, ..., \lambda_{nn}$ such that for a weight function $\omega : (a,b) \to \mathbb{R}, \omega(x) < 0$ , $x \in (a,b)$, 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

$$\lambda_{in} \;=\; \int_a^b \omega(x) \frac{p_{n+1}(x)}{(x \;-\; x_{in})\; p'_{n+1}(x_{in})}\, dx \;,\;\; 0 \le i \le n$$

there holds:

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

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,

$$p(x_{in}) \;=\; q(x_{in})\, p_{n+1}(x_{in}) \;+\; r(x_{in}) \;=\; r(x_{in}) \;,\;\; 0 \le i \le n \;.$$

Further, let

$$r \;=\; \sum_{i=0}^{n} r(x_{in})\, L_{in} \;=\; \sum_{i=0}^{n} p(x_{in})\, L_{in}$$

be the representation of $r$ as the Lagrangian interpolating polynomial with respect to the nodes $x_{0n}, ..., x_{nn}$. Then, there holds:

$$I(p) \;=\; \int_a^b \omega(x)\, p(x)\, dx \;=\; \underbrace{\int_a^b \omega(x)\, q(x)\, p_{n+1}(x)\, dx}_{=0} + \int_a^b \omega(x)\, r(x)\, dx \;=$$

$$= \sum_{i=0}^{n} p(x_{in}) \int_a^b \omega(x)\, L_{in}(x)\, dx \;.$$

Moreover, we have

$$L_{in}(x) \;=\; \prod_{k \neq i} \frac{x - x_{kn}}{x_{in} - x_{kn}} \;=\; \frac{p_{n+1}(x)}{x - x_{in}} \prod_{k \neq i} \frac{1}{x_{in} - x_{kn}} \;,$$

$$p'_{n+1}(x) \;=\; \Big[ \prod_{k=0}^{n} (x - x_{kn}) \Big]' \;=\; \sum_{j=0}^{n} \prod_{k \neq j} (x - x_{kn}) \quad \Longrightarrow \quad p'_{n+1}(x_{in}) \;=\; \prod_{k \neq i} (x_{in} - x_{kn}) \;,$$

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:

| Name of quadrature formula | $[a, b]$ | $\omega(\alpha, \beta)$ | $p_n$ |
|---|---|---|---|
| Gauss-Legendre | $[-1, +1]$ | $1$ | $P_n$ |
| Gauss-Chebyshev | $[-1, +1]$ | $(1 - x^2)^{-1/2}$ | $T_n$ |
| Gauss-Jacobi | $[-1, +1]$ | $(1 - x)^{\alpha}(1 + x)^{\beta}$ | $P_n^{(\alpha,\beta)}$ |
| Gauss-Laguerre | $[0, \infty)$ | $x^{\alpha}\exp(-x)$ | $L_n^{(\alpha)}$ |
| Gauss-Hermite | $(-\infty, +\infty)$ | $\exp(-x^2)$ | $H_n$ |

**Theorem 5.8 Approximation error**

Let $f \in C^{2n+2}([a,b])$, where $-\infty \le a < b \le +\infty$, and assume that $\max_{x\in[a,b]} |f^{(k)}(x)| < \infty \ , \ 0 \le k \le 2n+2$.

Then, there holds

$$| \, \hat{I}(f) \ - \ I(f) \, | \ \le \ (p_{n+1}, p_{n+1}) \ \max_{x\in[a,b]} \frac{| \, f^{(2n+2)}(x) \, |}{(2n+2)!} \ .$$

**Proof:** Let $\hat{f} \in P_{2n+1}([a,b])$ be the Hermitian interpolating polynomial with respect to $x_i, 0 \le i \le n$:

$$\hat{f}(x_i) \ = \ f(x_i) \quad , \quad \hat{f}'(x_i) \ = \ f'(x_i) \quad , \quad 0 \le i \le n \ .$$

$\hat{f}$ has the representation:

$$\hat{f}(x) \ = \ \sum_{i=0}^{n} (c_{in} \, x \ + \ d_{in}) \, L_{in}^2(x) \, f(x_{in}) \ + \ \sum_{i=0}^{n} (x \ - \ x_{in}) \, L_{in}^2(x) \, f'(x_{in}) \ ,$$

$$\text{with} \quad c_{in} \ := \ - \, 2 \prod_{j \ne i} \frac{1}{x_{in} \ - \ x_{jn}} \quad , \quad d_{in} \ := \ 1 \ - \ c_{in} \, x_{in} \ , \ 0 \le i \le n \ .$$

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 $\xi(x) \in (\min_{0 \le i \le n}(x, x_{in}), \max_{0 \le i \le n}(x, x_{in}))$. 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 $\Longrightarrow$ extrapolation method

### 5.3.1 Asymptotic expansion of the trapezoidal sum

We consider the trapezoidal sum

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

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

$$T(h) \ = \ \int_a^b f(x) \, dx \ + \ \sum_{k=1}^{m} \tau_{2k} \, h^{2k} \ + \ R_{2m+2}(h) \, h^{2m+2} \ .$$

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

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

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 $O(h^4)$:

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

We have:

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

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Numerical Analysis, Fall 2005

There holds:

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

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

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

We realize that $(\star)$ 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 $\tau_{kp}$ , $1 \le k \le m$, such that

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

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

$$p_{ik}(h^p) \;=\; p(h^p \mid h^p_{i-k+1}, ..., h^p_i) \text{ in } P_{k-1}(h^p)$$

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

$$T_{ik} \;=\; p_{ik}(0) \quad , \quad 1 \le k \le i \;.$$

According to the algorithm of Aitken-Neville, the values $T_{ik}$ can be computed recursively as follows:

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

$$T_{ik} = T_{i,k-1} + \frac{T_{i,k-1} - T_{i-1,k-1}}{\left(\frac{h_{i-k+1}}{h_i}\right)^p - 1} \quad , \quad 2 \le k \le i .$$

We thus obtain the extrapolation table:

$$\begin{array}{llllllll}
T_{11} & & & & & & & \\
T_{21} & T_{22} & & & & & & \\
\cdot & & \cdot & & & & & \\
\cdot & & & \cdot & & & & \\
\cdot & & & & \cdot & & & \\
T_{k-1,1} & \cdot & \cdot & \cdot & \cdot & \cdot & T_{k-1,k-1} & \\
T_{k,1} & \cdot & \cdot & \cdot & \cdot & \cdot & T_{k,k-1} & T_{k,k}
\end{array}$$

Denoting the approximation error with respect to $T_{ik}$ by

$$\varepsilon_{ik} := - \tau_0 \,\Big| \quad , \quad 1 \le k \le i \,,$$

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 $T_{ik}$ , $1 \le k \le i \le m$, be the approximations computed by extrapolation to the steplength $h = 0$ with respect to the steplengths $h_j$ , $1 \le j \le m$.
Then, for the extrapolation error there holds

$$\varepsilon_{ik} = |\tau_{kp}| \prod_{j=i-k+1}^{i} h_j^p + \sum_{j=i-k+1}^{i} O(h_j^{(k+1)p}) \quad , \quad (h_j \le h \to 0) \,.$$

Proof: By assumption, for $1 \le k \le m$ there holds:

$$(\bullet) \quad T_{j1} \;=\; T(h_j) \;=\; \tau_0 \;+\; \sum_{\ell=1}^{k} \tau_{\ell p}\, h_j^{\ell p} \;+\; O(h_j^{(k+1)p}) \;.$$

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

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

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

$$\sum_{j=1}^{k} L_j(0)\, h_j^{\ell p} \;=\; \begin{cases} 1 & , \quad \ell = 0 \\ 0 & , \quad 1 \le \ell \le k-1 \\ (-1)^{k-1} \prod\limits_{\nu=1}^{k} h_\nu^p & , \quad \ell = k \end{cases}$$

and observing $(\bullet)$, 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 $1 \le k < i$ are shown analogously.

### 5.3.3 Implementation of the Romberg integration

The application of the previously described extrapolation technique to the numerical computation 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

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

Once $n_i \ , \ i = 0, 1, 2, ...$ has been specified, the method is characterized by the sequence of steplengths

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

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

$$\mathcal{A} = \{A_0, A_1, ...\} \ .$$

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:

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

If we observe

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

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

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

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 compu--tational work:

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

whence

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

The associated sequence of computational work is given by:

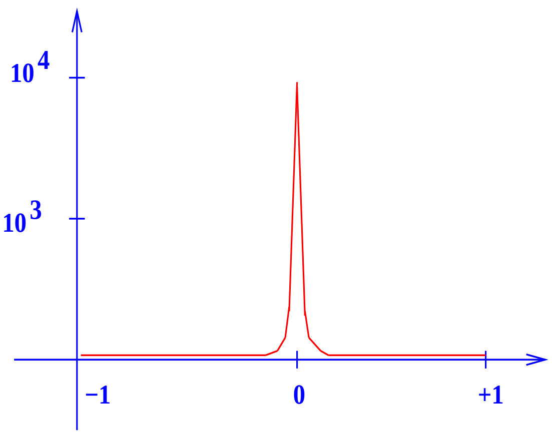
$$\mathcal{A}_B = \{2, 3, 7, 9, 13, 17, ...\} \, .$$

## 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 $\Delta^i$ 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

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

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

$$(\mathrm{S}) \quad \Big|\, S(J) - \int_{x_\ell}^{x_r} f(x)\,dx \,\Big| \le q_J \,\Big|\, T(J) - \int_{x_\ell}^{x_r} f(x)\,dx \,\Big| \quad , \quad 0 \le q_J < 1$$

there holds:

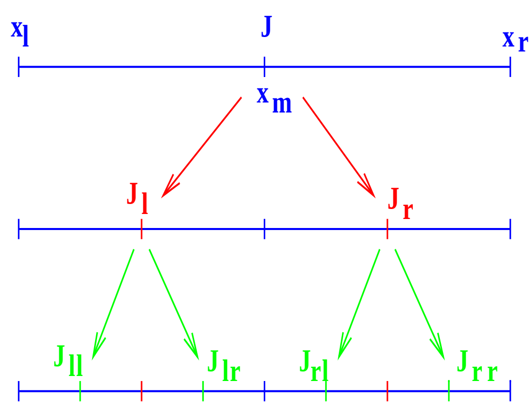
$$(\diamond) \quad \frac{1}{1+q_J}\,\big|\, T(J) - S(J) \,\big| \le \Big|\, \int_{x_\ell}^{x_r} f(x)\,dx - T(J) \,\Big| \le \frac{1}{1-q_J}\,\big|\, T(J) - S(J) \,\big| \,,$$

i.e., the quantity

$$(\star) \quad \bar{\varepsilon}(J) := \big|\, T(J) - S(J) \,\big|$$

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 $\mathbf{J}_\ell$ as the father of $\mathbf{J}_{\ell\ell}$ and $J_{\ell_r}$ as well as the son of $\mathbf{J}$. In the following, we denote the father of an interval $\mathbf{J}$ by $\mathbf{J}^-$.

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

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

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

Therefore, we are interested in another error estimator $\varepsilon^+(\mathbf{J})$ which provides information about the error $\varepsilon(\mathbf{J}_\ell)$ of the next level in case $\mathbf{J}$ has been partitioned into $\mathbf{J}_\ell$ and $\mathbf{J}_\mathrm{r}$.

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

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

We thus obtain:

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

Consequently, the quantity

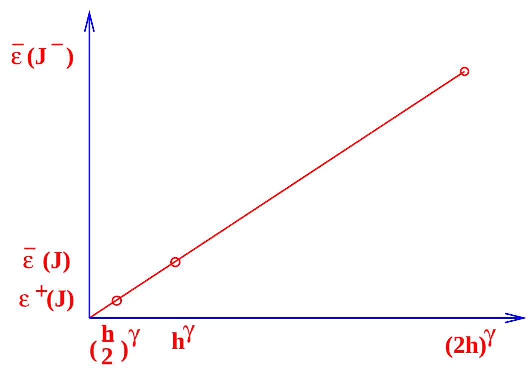
$$\varepsilon^{+}(J) := \frac{\bar{\varepsilon}(J)^2}{\bar{\varepsilon}(J^-)}$$

may serve as the required error estimator.

The error estimator

$$\varepsilon^+(\mathbf{J}) \;:=\; \frac{\bar{\varepsilon}(\mathbf{J})^2}{\bar{\varepsilon}(\mathbf{J}^-)}$$

can be interpreted in the local extrapolation.




We define:

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

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

$$\bar{\varepsilon}(\mathbf{J}) \;\geq\; \kappa(\Delta)\;.$$