2 Numerical integration

<u>Goal:</u> determine (approximately) $\int_a^b f(x)\,dx$
Quadratur formelas: We consider quadrature formulas of the form

$$\int_a^b f(x)\,dx \approx Q_a^b(f) = \sum_{i=0}^{n} w_i f(x_i) \tag{2.1}$$

The points x_i are called *quadratur points*, the numbers ω_i *quadratur weights.*

Example 2.1 **slide 10**
Partition $[a,b]$ *in* N *subintervals* $[t_i, t_{i+1}]$, $i = 0,\ldots,N-1$ *with* $t_i = a + ih$, $h = (b-a)/N$. *Let* $m_i := (t_i + t_{i+1})/2$ *be the midpoints. Then the* composite midpoint rule *is*

$$\int_a^b f(x)\,dx \approx Q_a^b(f) = \sum_{i=0}^{N-1} h f(m_i)$$

∎

Example 2.2 *The* (composite) trapezoidal *rule is given, with the notation of Example 2.1, by*

$$\int_a^b f(x)\,dx \approx Q_a^b(f) = \sum_{i=0}^{N-1} h\frac{1}{2}\left[f(t_i) + f(t_{i+1})\right] = h\left[\frac{1}{2}f(a) + \sum_{i=1}^{N-1} f(t_i) + \frac{1}{2}f(b)\right].$$

∎

The Examples 2.1, 2.2 are typical representatives for the way composite quadrature rules are generated:

1. define a quadrature rule $\widehat{Q}(f) \approx \int_0^1 f(x)\,dx$ on a reference interval, e.g., $[0,1]$.
2. Partition the interval $[a,b]$ in subintervals (t_i, t_{i+1}) of lengths $h_i = t_{i+1} - t_i$
3. The observation $\int_{t_i}^{t_{i+1}} f(x)\,dx = h_i \int_0^1 f(t_i + h_i\xi)\,d\xi$ motivates the definition

$$\int_a^b f(x)\,dx = \sum_{i=0}^{N-1} \int_{t_i}^{t_{i+1}} f(x)\,dx = \sum_{i=0}^{N-1} h_i \int_0^1 f(t_i + h_i\xi)\,d\xi \approx \sum_{i=0}^{N-1} h_i \widehat{Q}(f(t_i + h_i\cdot))$$

Remark 2.3 *Quadrature rules are normally formulated for a reference interval, which is typically* $[0,1]$ *or* $[-1,1]$. *For a general interval* $[a,b]$, *the rule is obtained by an affine change of variables (as done above).* ∎

2.1 Newton-Cotes formulas

The Newton-Cotes formulas for the integration on $[0,1]$ are examples of *interpolatory* quadrature formulas. They are based on interpolating the integrand f and integrating the intepolating polynomial. The interpolation points are uniformly distributed over $[0,1]$.

Example 2.4 (closed Newton-Cotes formulas) *Let $n \geq 1$ and $x_i = \frac{i}{n}$, $i = 0,\dots,n$. The interpolating polynomial $p \in \mathcal{P}_n$ is*

$$p(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x), \qquad \ell_i(x) = \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}.$$

Hence, the quadrature fromula is

$$\int_0^1 f(x)\,dx \approx \int_0^1 p(x)\,dx = \int_0^1 \sum_{i=0}^{n} f(x_i)\ell_i(x)\,dx = \sum_{i=0}^{n} f(x_i) \underbrace{\int_0^1 \ell_i(x)\,dx}_{=:w_i} =: \widehat{Q}_n^{cNC}(f)$$

with the quadrature weights w_i, $i = 0,\dots,n$, which are explicitly given in Fig. 2.1. ∎

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The endpoints of the interval are quadrature points for the "closed" formulas of Example 2.4. If, for example, integrands are not defined at an endpoint (e.g., $1/\sqrt{x}$, $\log x$), then it is more convenient to have formulas that do not sample the integrand at the endpoint. Hence, another very important class of Newton-Cotes formulas are the "open" formulas:

Example 2.5 (open Newton-Cotes-Formeln) *Let $n \geq 0$ and $x_i = \frac{2i+1}{2n+2}$, $i = 0,\dots,n$. Then the quadrature is given by*

$$\int_0^1 f(x)\,dx \approx \sum_{i=0}^{n} f(x_i) \underbrace{\int_0^1 \ell_i(x)\,dx}_{=:w_i} =: \widehat{Q}_n^{oNC}(f), \qquad \ell_i(x) = \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}.$$

The choice $n = 0$ corresponds to the midpoint rule

$$\int_0^1 f(x)\,dx \approx Q^{mid}(f) = f(1/2).$$

By construction the Newton-Cotes formulas are exact for polynomials $f \in \mathcal{P}_n$. In fact, one can show that, if n is even, then both the closed and the open Newton-Cotes formulas are exact for polynomials $f \in \mathcal{P}_{n+1}$.

Exercise 2.6

1. *Show for the quadrature weights: $\sum_{i=0}^{n} w_i = 1$(= length of the interval $[0,1]$) (*hint: *apply the quadrature formula to a suitable function f.)*
2. *Show that the quadrature formulas $\widehat{Q}_n^{cNC}$, $\widehat{Q}_n^{oNC}$ are exact for $f \in \mathcal{P}_n$.*
3. *Show the symmetry property $w_{n-i} = w_i$, $i = 0,\dots,n$. (*hint: *Use the symmetry of the points with respect to $1/2$. The symmetry of the weights is visible in Fig. 2.1.).*

n	weight	$Q(f) - \int_0^1 f(x)\,dx$	name
1	$\frac{1}{2}$ $\frac{1}{2}$	$\frac{1}{12}h^3 f^{(2)}(\xi)$	trapezoidal rule
2	$\frac{1}{6}$ $\frac{4}{6}$ $\frac{1}{6}$	$\frac{1}{90}h^5 f^{(4)}(\xi)$	Simpson rule
3	$\frac{1}{8}$ $\frac{3}{8}$ $\frac{3}{8}$ $\frac{1}{8}$	$\frac{3}{80}h^5 f^{(4)}(\xi)$	3/8 rule
4	$\frac{7}{90}$ $\frac{32}{90}$ $\frac{12}{90}$ $\frac{32}{90}$ $\frac{7}{90}$	$\frac{8}{945}h^7 f^{(6)}(\xi)$	Milne rule
5	$\frac{19}{288}$ $\frac{75}{288}$ $\frac{50}{288}$ $\frac{50}{288}$ $\frac{75}{288}$ $\frac{19}{288}$	$\frac{275}{12096}h^7 f^{(6)}(\xi)$	—
6	$\frac{41}{840}$ $\frac{216}{840}$ $\frac{27}{840}$ $\frac{272}{840}$ $\frac{27}{840}$ $\frac{216}{840}$ $\frac{41}{840}$	$\frac{9}{1400}h^9 f^{(8)}(\xi)$	Weddle rule

Figure 2.1: the closed Newton-Cotes formulas for the integration over $[0,1]$. Quadrature points are $x_i = \frac{i}{n}$, $i = 0, \ldots, n$; $h = \frac{1}{n}$.

4. *Let $n = 2m$ be even. Consider the function $f = (x - 1/2)^{n+1}$, which is odd with respect to 1/2. Show: $\int_0^1 f(x)\,dx = 0 = \widehat{Q}_n^{cNC}(f) = \widehat{Q}_n^{oNC}(f)$. Conclude that the quadrature formula is exact for polynomials of degree $n+1$. In particular, the midpoint rule is exact for polynomials in $\mathcal{P}_1$, and the Simpson rule is exact for polynomials in $\mathcal{P}_3$.* ∎

The Newton-Cotes formulas are typically used for fixed n in composite rule. We illustrate the convergence behavior for two important cases, the composite trapezoidal rule and the composite Simpson rule. Let $a = x_0 < x_1 < \ldots < x_N = b$ be a partition of $[a,b]$ and $h_i := x_{i+1} - x_i$. Then the composite trapezoidal and Simpson rules are defined by

$$T_{\{x_0,\ldots,x_N\}}(f) := \sum_{i=0}^{N-1} h_i \frac{1}{2}\left(f(x_i) + f(x_{i+1})\right),$$

$$S_{\{x_0,\ldots,x_N\}}(f) := \sum_{i=0}^{N-1} h_i \frac{1}{6}\left(f(x_i) + 4f(\frac{x_i + x_{i+1}}{2}) + f(x_{i+1})\right).$$

Theorem 2.7 *(i) Let $f \in C([a,b])$. Then:*

$$\left|\int_a^b f(x)\,dx - T_{\{x_0,\ldots,x_N\}}(f)\right| \le 2\sum_{i=0}^{N-1} h_i \min_{v\in\mathcal{P}_1} \|f - v\|_{\infty,[x_i,x_{i+1}]},$$

$$\left|\int_a^b f(x)\,dx - S_{\{x_0,\ldots,x_N\}}(f)\right| \le 2\sum_{i=0}^{N-1} h_i \min_{v\in\mathcal{P}_3} \|f - v\|_{\infty,[x_i,x_{i+1}]}.$$

(ii) Let $f \in C^2([a,b])$. Then for $h := \max_{i=0,\ldots,N-1} h_i$

$$\left|\int_a^b f(x)\,dx - T_{\{x_0,\ldots,x_N\}}(f)\right| \le \frac{1}{4}\sum_{i=0}^{N-1} h_i^3 \|f^{(2)}\|_{\infty,[x_i,x_{i+1}]} \le \frac{1}{4}(b-a)h^2\|f^{(2)}\|_{\infty,[a,b]}$$

(iii) Let $f \in C^4([a,b])$. Then for $h := \max_{i=0,\ldots,N-1} h_i$ with a constant $C > 0$

$$\left|\int_a^b f(x)\,dx - S_{\{x_0,\ldots,x_N\}}(f)\right| \le C\sum_{i=0}^{N-1} h_i^5 \|f^{(4)}\|_{\infty,[x_i,x_{i+1}]} \le C(b-a)h^4\|f^{(4)}\|_{\infty,[a,b]}$$

Proof: We only prove the case of the trapezoidal rule—the assertion for the Simpson rule is proved using similar techniques.
We denote by $T_{\{x_i,x_{i+1}\}}(f) = h_i \frac{1}{2}(f(x_i) + f(x_{i+1}))$ the trapezoidal rule for the interval $[x_i, x_{i+1}]$. This rule is exact for polynomials of degree $n = 1$. Hence, for arbitrary $v \in \mathcal{P}_1$

$$\begin{aligned}
\int_{x_i}^{x_{i+1}} f(x)\,dx - T_{\{x_i,x_{i+1}\}}(f) &= \int_{x_i}^{x_{i+1}} f(x) - v(x)\,dx + \int_{x_i}^{x_{i+1}} v(x)\,dx - T_{\{x_i,x_{i+1}\}}(f) \\
&= \int_{x_i}^{x_{i+1}} f(x) - v(x)\,dx + T_{\{x_i,x_{i+1}\}}(v) - T_{\{x_i,x_{i+1}\}}(f) \\
&= \int_{x_i}^{x_{i+1}} f(x) - v(x)\,dx - T_{\{x_i,x_{i+1}\}}(f - v).
\end{aligned}$$

Therefore,

$$\begin{aligned}
\left| \int_{x_i}^{x_{i+1}} f(x)\,dx - T_{\{x_i,x_{i+1}\}}(f) \right| &\le (x_{i+1} - x_i)\|f - v\|_{\infty,[x_i,x_{i+1}]} + |T_{\{x_i,x_{i+1}\}}(f - v)| \\
&\le (x_{i+1} - x_i)\|f - v\|_{\infty,[x_i,x_{i+1}]} + (x_{i+1} - x_i)\|f - v\|_{\infty,[x_i,x_{i+1}]} \\
&\le 2h_i\|f - v\|_{\infty,[x_i,x_{i+1}]}.
\end{aligned}$$

Hence,

$$\left| \int_a^b f(x) - T_{\{x_0,\ldots,x_N\}}(f) \right| = \left| \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x)\,dx - T_{\{x_i,x_{i+1}\}}(f) \right| \le \sum_{i=0}^{N-1} 2h_i \min_{v \in \mathcal{P}_1} \|f - v\|_{\infty,[x_i,x_{i+1}]}$$

which is the statement (i) for the trapezoidal rule. In order to conclude (ii), we select for each subinterval $[x_i, x_{i+1}]$ a polynomial $v \in \mathcal{P}_1$ that approximates f on $[x_i, x_{i+1}]$ well, e.g., the linear interpolant. From the error bound of Theorem 1.15 we obtain

$$\min_{v \in \mathcal{P}_1} \|f - v\|_{\infty,[x_i,x_{i+1}]} \le \frac{1}{8}(x_{i+1} - x_i)^2 \|f''\|_{\infty,[x_i,x_{i+1}]},$$

from which we arrive at

$$\left| \int_a^b f(x) - T_{\{x_0,\ldots,x_N\}}(f) \right| \le \frac{1}{4} \sum_{i=0}^{N-1} h_i^3 \|f''\|_{\infty,[x_i,x_{i+1}]}$$

With $h_i \le h$ we finally get

$$\begin{aligned}
\left| \int_a^b f(x) - T_{\{x_0,\ldots,x_N\}}(f) \right| &\le \frac{1}{4} \sum_{i=0}^{N-1} h_i^3 \|f''\|_{\infty,[x_i,x_{i+1}]} \le \frac{1}{4} h^2 \sum_{i=0}^{N-1} h_i \|f''\|_{\infty,[x_i,x_{i+1}]} \\
&\le \frac{1}{4} h^2 \|f''\|_{\infty,[a,b]} \sum_{i=0}^{N-1} h_i = \frac{1}{4} h^2 \|f''\|_{\infty,[a,b]} (b - a).
\end{aligned}$$

□

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We say that a quadrature rule has *order* m if the the composite rule leads to error bounds of the form Ch^m (for sufficiently smooth f). Die composite trapezoidal rule has therefore order $m = 2$, the composite Simpson rule order $m = 4$. More generally, the proof of Theorem 2.7 shows that a Newton-Cotes formula (or, more generally, any composite rule) that is exact for polynomials of degree n leads to a composite rule of order $n + 1$.

h	2^0	2^{-1}	2^{-2}	2^{-3}	2^{-4}	2^{-5}	2^{-6}	2^{-7}	2^{-8}
$F_{trap} \sim 1/h$	2	3	5	9	17	33	65	129	257
E_{trap}	1.4_{-1}	3.6_{-2}	8.9_{-3}	2.2_{-3}	5.6_{-4}	1.4_{-4}	3.5_{-5}	8.7_{-6}	2.2_{-6}
$F_{Simpson} \sim 1/h$	3	5	9	17	33	65	129	257	513
$E_{Simpson}$	5.8_{-4}	3.7_{-5}	2.3_{-6}	1.5_{-7}	9.1_{-9}	5.7_{-10}	3.6_{-11}	2.2_{-12}	1.4_{-13}

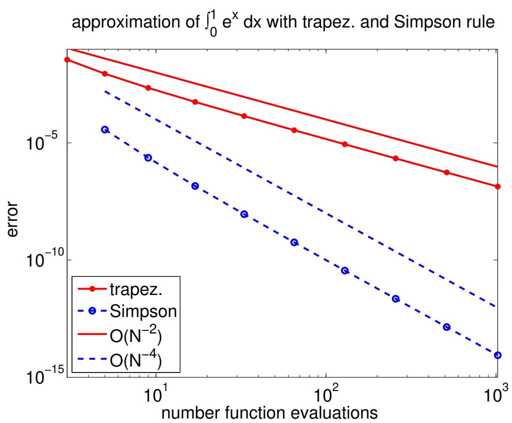

Figure 2.2: convergence behavior of composite trapezoidal and Simpson rule for smooth integrand.

Example 2.8 slide 12
We compare the composite trapezoidal rule with the composite Simpson rule for integration on $[0,1]$. *We partition* $[0,1]$ *in* N *subintervals of length* $h = 1/N$. *By Theorem 2.7 the errors* E_{trap}, $E_{Simpson}$ *satisfy (*F *denotes the number of function evaluations):*

$$E_{trap}(h) \leq Ch^2 \sim CF^{-2}, \qquad E_{Simpson} \leq Ch^4 \sim CF^{-4}.$$

We show in Fig. 2.2 the error versus the number of function evaluations F*, since this is a reasonable cost measure of the method. We note that methods of a higher order are more efficient than lower order methods.* ∎

Das $O(h^2)$ convergence behavior of the composite trapezoidal rule and the $O(h^4)$ behavior of the compositive Simpson rule require $f \in C^2$ and $f \in C^4$, respectively:

Example 2.9 *Integration of* $f(x) = x^{0.1}$ *on* $[0,1]$ *does* not *yield* $O(h^2)$ *but merely* $O(h^{1.1})$ *as is visible on*
slide 12
.

2.2 Romberg extrapolation

Extrapolation can be used to accelerate convergence of composite rules for smooth integrands. We illustrate the procedure for the composite trapezoidal rule. For that, let the interval $[a,b]$ be partitioned in N subintervals (x_i, x_{i+1}) of length $h = (b-a)/N$ with $x_i = a + ih$. Define

$$T(h) := h \sum_{i=0}^{N-1} \frac{1}{2} \left(f(x_i) + f(x_{i+1})\right)$$

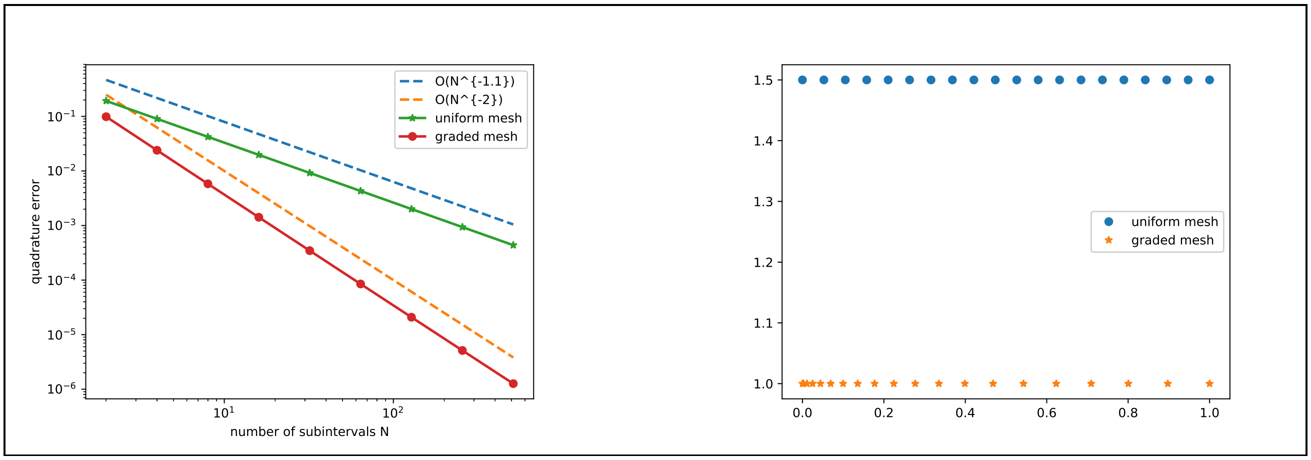

Figure 2.3: (cf. Example 2.11) numerical integration of $f(x) = x^{0.1}$ using composite trapezoidal rule based on a) equidistant nodes and b) nodes suitable refined towards $x = 0$.

The sought value of the integral $\int_a^b f(x)\,dx = \lim_{h\to 0} T(h)$, so that one may use extrapolation for the data $(h_i, T(h_i))$, $i = 0, 1, \ldots$, with $h_i = (b-a)M^{-i}$ for some chosen $M \in \mathbb{N}$, $M \geq 2$.[1] In fact, $T(h)$ has an "additional structure" (cf. Section 1.6): There holds (reference!):

$$T(h) = \int_a^b f(x)\,dx + c_1 h^2 + c_2 h^4 + c_3 h^6 + \cdots, \tag{2.2}$$

where the coefficients c_i depend on higher derivatives of f. Therefore, one will perform extrapolation as discussed in Section 1.6.
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Remark 2.10 *Extrapolation of the composite trapezoidal rule for $M = 2$ yields in the first columns of the Neville scheme the composite Simpson rule; in the second column, the composite Milne rule arises. The choice $M = 3$ produces in the first column of the Neville scheme the composite 3/8-rule.* ■

2.3 non-smooth integrands and adaptivity

Example 2.9 shows that, for non-smooth integrands, composite quadrature rules based on equidistant partitions $x_0 < x_1 < \cdots < x_N$ do not work very well. Our goal is a choose the partition in such a way that the composite trapezoidal rule yields convergence $O(N^{-2})$, where N is the number of quadrature points. In other words: the convergence (error vs. number of function evaluations) is similar to the case of smooth integrands.
This can be achieved for quite a few integrands f if the partition is suitably adapted to f. Basically, one should use small interval lengths h_i where f is large (in absolute value) or varies rapidly (i.e., higher derivatives of f are large):

Example 2.11 **slide 14**
Consider the composite trapezoidal rule for $\int_0^1 f(x)\,dx$ mit $f(x) = x^{0.1}$ for two partitions of $0 = x_0 < x_1 \cdots < x_N = 1$ of the form

[1] strictly speaking, $T(h)$ is only defined for h of the form $h = (b-a)/N$, $N \in \mathbb{N}$, so that one should write $\int_a^b f(x)\,dx = \lim_{N\to\infty} T(h(N))$.

1. equidistant points: $x_i = (i/N)$, $i = 0, \ldots, N$

2. points refined towards $x = 0$*:* $x_i = (i/N)^\beta$, $i = 0, \ldots, N$ *mit* $\beta = 2$

The convergence behavior of the composite trapezoidal rule is shown in Fig. 2.3. While the convergence is only $O(N^{-1.1})$ *for the equidistant points, it is* $O(N^{-2})$ *for the one where the points are refined towards* $x = 0$*.* ∎

In practice, it is difficult to construct a good partition for a given integrand. One is therefore interested in *adaptive algorithms*. Structurally, these algorithms proceed as outlined in Algorithm 2.12: the accuracy of an approximation for the integration on an interval $[a, b]$ (here: using the trapezoidal rule) is estimated with a better rule (here: Simpson rule). If the estimate accuracy does not meet the desired tolerance, then the interval $[a, b]$ is subdivided into two subintervals $[a, m]$, $[m, b]$ with midpoint $m = (a+b)/2$ and the quadrature routine is recursively call for the two subintervals.

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Algorithm 2.12 (adaptive algorithm based on trapezoidal rule)

adapt*(f,a,b,τ)*

% approximates $\int_a^b f(x)\,dx$ *to given accuracy* τ
% h_{min} *= minimal interval length ;* $\rho \in (0, 1)$ *safety factor*
% $T([a, b])$ *= trapezoidal rule für* $[a, b]$*;* $S([a, b])$ *= Simpson rule for* $[a, b]$
if $(b - a) \leq h_{min}$ **return**$(S([a, b]))$ *%forced termination!*
if $|S([a, b]) - T([a, b])| \leq \rho\tau$ { *desired accuracy reached :)*
  return *(S([a,b]))* }
else {
%desired accuracy not reached $\rightarrow$ *subdived* $[a, b]$ *into* $[a, m]$ *and* $[m, b]$
$m := (a + b)/2$
$I :=$ **adapt**$(f, a, m, \tau/2) +$ **adapt**$(f, m, b, \tau/2)$
return*(I)* }

2.4 Gaussian quadrature

Question: How to choose $n + 1$ quadrature points so that polynomials of the highest possible degree are integrated exactly?
Answer: Gaussian quadrature integrates polynomials of degree $2n + 1$ exactly. The $n + 1$ quadrature points ("Gaussian points") of this quadrature rule are the zeros of the Legendre polynomial L_{n+1}.