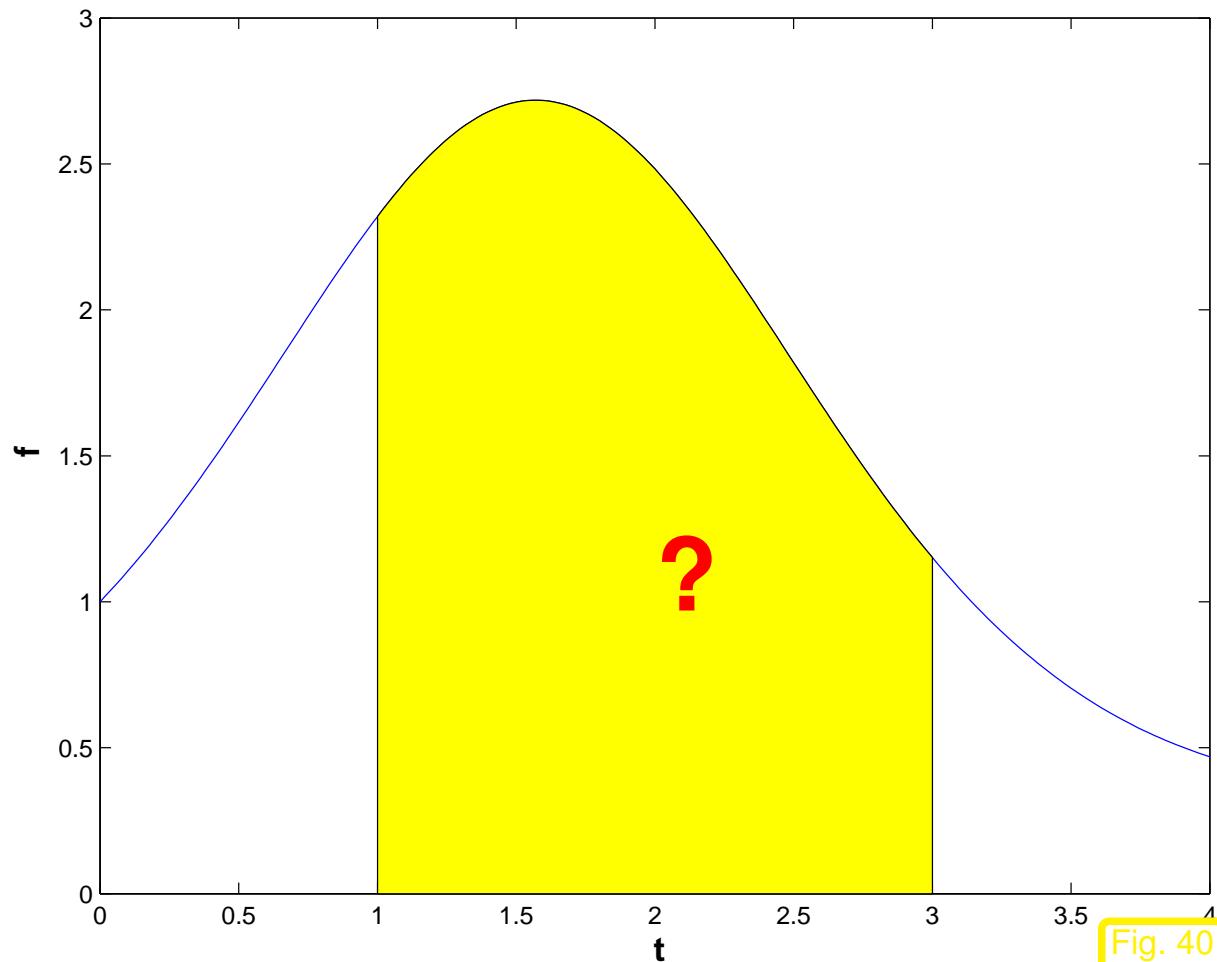


7

Numerical Quadrature



Numerical quadrature methods

approximate

$$\int_a^b f(t) dt$$

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7.1 Quadrature Formulas

Definition 7.1.1. Let $-\infty < a < b < \infty$, let $n \in \mathbb{N}$, let $w_1, \dots, w_n \in \mathbb{R}$ and let $c_1, \dots, c_n \in [a, b]$. Then a function $Q: \{f: [a, b] \rightarrow \mathbb{R}\} \rightarrow \mathbb{R}$ satisfying

$$Q(f) = \sum_{j=1}^n w_j f(c_j) \quad (7.1.1)$$

for all functions $f: [a, b] \rightarrow \mathbb{R}$ is called **quadratur formula** (on $[a, b]$ with **quadrature weights** (ger.: Quadraturgewichte) w_1, \dots, w_n and **quadrature nodes** (ger.: Quadraturknoten) c_1, \dots, c_n).

Notation: In the following we denote by $Q_{c_1, \dots, c_n, [a, b]}^{w_1, \dots, w_n}: \{f: [a, b] \rightarrow \mathbb{R}\} \rightarrow \mathbb{R}$ the quadrature formula on $[a, b]$ with quadrature weights w_1, \dots, w_n and quadrature nodes c_1, \dots, c_n , i.e., the function given by (7.1.1).

Finally, if there are $m \in \mathbb{N}$, $a \leq \hat{c}_1 < \dots < \hat{c}_m \leq b$ and $\hat{w}_1, \dots, \hat{w}_m \in \mathbb{R} \setminus \{0\}$ such that $Q = Q_{\hat{c}_1, \dots, \hat{c}_m, [a, b]}^{\hat{w}_1, \dots, \hat{w}_m}$, then we say that Q is an **m -point quadrature formula**.

$t_1, \dots, t_n \in [a, b]$ of a quadrature formula Q on $[a, b]$ are chosen so that

$$Q(f) = \sum_{j=1}^n w_j f(c_j) \approx \int_a^b f(t) dt \quad (7.1.2)$$

in an appropriate sense for integrable functions $f: [a, b] \rightarrow \mathbb{R}$.

Note that the number $n \in \mathbb{N}$ of nodes agrees with the number of f -evaluations required for one evaluation of the quadrature formula. This is usually used as a *measure for the cost* of computing $Q(f)$.

Inevitable for generic integrand: **Quadrature error**.

If Q is a quadrature formula on $[a, b]$ and if $f: [a, b] \rightarrow \mathbb{R}$ is an integrable function, then we denote by $E_Q(f)$ the **quadrature error** of Q for f given by

$$E_Q(f) := \left| \int_a^b f(t) dt - Q(f) \right| .$$

Definition 7.1.2 (Order of a quadrature formula). Let $-\infty < a < b < \infty$ and let $k \in \mathbb{N}$. A quadrature formula Q on $[a, b]$ is said to be of order k if

$$E_Q(f|_{[a,b]}) = 0 \quad (7.1.3)$$

for all polynomials $f \in \mathcal{P}_{k-1}$ with degree $\leq k-1$.

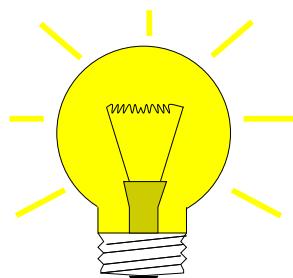
Remark 7.1.1 (Transformation of quadrature formulas). Let $n, k \in \mathbb{N}$, let $w_1, \dots, w_n \in \mathbb{R}$, let $c_1, \dots, c_n \in [a, b]$, let $-\infty < a < b < \infty$ and $-\infty < \hat{a} < \hat{b} < \infty$ and consider the quadrature formula

$$f \mapsto Q_{c_1, \dots, c_n, [a, b]}^{w_1, \dots, w_n}(f) = \sum_{j=1}^n w_j f(c_j) \quad (7.1.4)$$

on $[a, b]$. Then we call the quadrature formula

$$f \mapsto Q_{\hat{a} + \frac{(c_1-a)}{(b-a)}(\hat{b}-\hat{a}), \dots, \hat{a} + \frac{(c_n-a)}{(b-a)}(\hat{b}-\hat{a}), [\hat{a}, \hat{b}]}^{w_1 \frac{\hat{b}-\hat{a}}{b-a}, \dots, w_n \frac{\hat{b}-\hat{a}}{b-a}}(f) = \frac{(\hat{b} - \hat{a})}{(b - a)} \left[\sum_{j=1}^n w_j f\left(\hat{a} + \frac{(c_j - a)}{(b - a)}(\hat{b} - \hat{a})\right) \right] \quad (7.1.5)$$

on $[\hat{a}, \hat{b}]$ the transformation of (7.1.4) to $[\hat{a}, \hat{b}]$. It holds that (7.1.4) is of order k if and only if (7.1.5) is of order k .

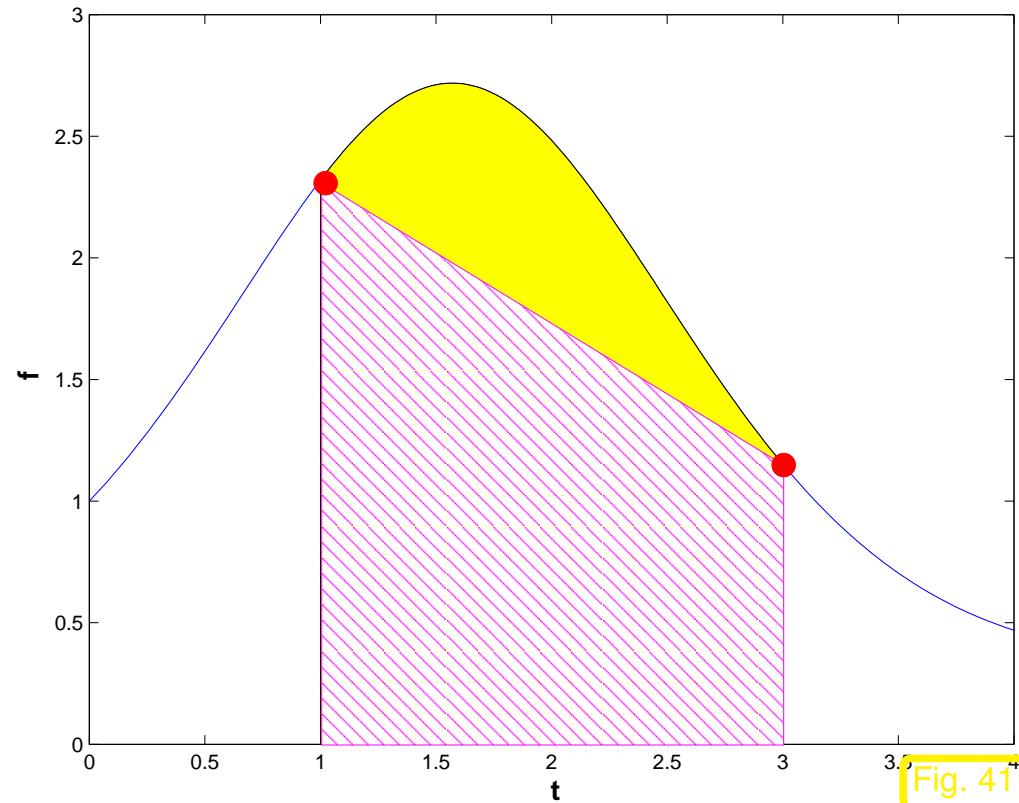


Closed Newton-Cotes formulas: Equidistant quadrature nodes $c_j := a + h(j - 1)$, $h := \frac{b-a}{n-1}$, $j \in \{1, 2, \dots, n\}$, $n \in \{2, 3, \dots\}$: choose the n quadrature weights for the quadrature formula $Q = Q_{c_1, \dots, c_n, [a, b]}^{w_1, \dots, w_n}$ such that Q is of order n , i.e., such that $E_Q(f|_{[a, b]}) = 0$ for all polynomials $f \in \mathcal{P}_{n-1}$ of degree $\leq n - 1$.

Example 7.1.2 (Closed Newton-Cotes formulas in the case $n = 2$ and $n = 3$).

- $n = 2$: Trapezoidal rule on $[a, b]$ (2-point quadrature formula of order 2):

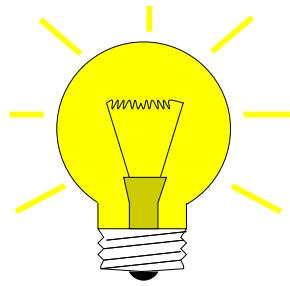
$$\int_a^b f(t) dt \approx \frac{(b-a)}{2} \left(f(a) + f(b) \right) = Q_{a, b, [a, b]}^{\frac{b-a}{2}, \frac{b-a}{2}}(f) \quad (7.1.7)$$



- $n = 3$: Simpson rule on $[a, b]$ (3-point quadrature formula of order 3):

$$\int_a^b f(t) dt \approx \frac{(b-a)}{6} \left(f(a) + 4 f\left(\frac{a+b}{2}\right) + f(b) \right) = Q_{a, \frac{a+b}{2}, b, [a,b]}^{\frac{b-a}{6}, \frac{2(b-a)}{3}, \frac{b-a}{6}}(f) \quad (7.1.8)$$

◇



Gaussian quadrature: Choose the $n \in \mathbb{N}$ quadrature weights and the n quadrature nodes of the quadrature formula $Q = Q_{c_1, \dots, c_n, [a, b]}^{w_1, \dots, w_n}$ such that Q is of order $2n$, i.e., such that $E_Q(f|_{[a, b]}) = 0$ for all polynomials $f \in \mathcal{P}_{2n-1}$ of degree $\leq 2n - 1$.

Example 7.1.4 (Gaussian quadrature in the case $n = 1$). Midpoint rule on $[a, b]$ (1-point quadrature formula of order 2):

$$\int_a^b f(t) dt \approx (b - a) f\left(\frac{a+b}{2}\right) = Q_{\frac{a+b}{2}, [a, b]}^{b-a}(f). \quad (7.1.10)$$

◇

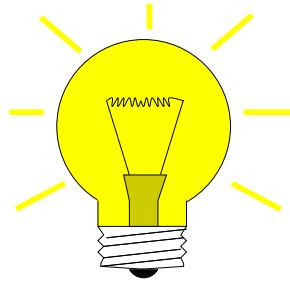
Example 7.1.5 (Gaussian quadrature in the case $n = 2$). 2-point quadrature formula of order 4: In the special case $a = -1$ and $b = 1$, i.e., $[a, b] = [-1, 1]$:

$$\int_{-1}^1 f(x) dx \approx f\left(\frac{1}{\sqrt{3}}\right) + f\left(-\frac{1}{\sqrt{3}}\right) = Q_{-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, [-1, 1]}^{1, 1}(f) \quad (7.1.11)$$

The general case follows from Remark 7.1.1.

◇

The quadrature nodes and the quadrature weights for higher order Gaussian quadrature formulas (that is, $n \in \{3, 4, \dots\}$) can be found in the literature (see, e.g., http://en.wikipedia.org/wiki/Gaussian_quadrature) or can be computed efficiently with the Golub-Welsch algorithm (see, e.g., [5, Sect. 3.5.4] or http://en.wikipedia.org/wiki/Gaussian_quadrature).



Idea of the **Clenshaw-Curtis** quadrature: Let $f: [-1, 1] \rightarrow \mathbb{R}$ be a smooth function.

Define $F: [0, \pi] \rightarrow \mathbb{R}$ through $F(\theta) := f(\cos(\theta))$ for all $\theta \in [0, \pi]$ and $a_k \in \mathbb{R}$, $k \in \mathbb{N}_0$, by

$$\forall k \in \mathbb{N}_0: \quad a_k = \begin{cases} \frac{2}{\pi} \int_0^\pi F(\theta) \cos(k\pi) d\theta & : k \in \mathbb{N} \\ \frac{1}{\pi} \int_0^\pi F(\theta) d\theta & : k = 0 \end{cases}. \quad (7.1.12)$$

Then $F(\theta) = \sum_{k=0}^{\infty} a_k \cos(k\theta)$ for all $\theta \in [0, \pi]$ and therefore

$$\begin{aligned} \int_{-1}^1 f(x) dx &= \int_0^\pi f(\cos \theta) \sin(\theta) d\theta = \int_0^\pi F(\theta) \sin(\theta) d\theta \\ &= \int_0^\pi \left[\sum_{k=0}^{\infty} a_k \cos(k\theta) \right] \sin(\theta) d\theta = \sum_{k=0}^{\infty} a_k \left[\int_0^\pi \cos(k\theta) \sin(\theta) d\theta \right] = \sum_{k=0}^{\infty} \frac{2a_{2k}}{(1 - 4k^2)} \end{aligned} \quad (7.1.13)$$

Advantage for the Clenshaw-Curtis quadrature is the speed and stability of the fast Fourier transform.

Equal spacing is a disaster for high-order interpolation and integration !

- Divide the integration domain in small pieces and use low-order rule on each piece: Composite quadrature!

- Take into account the eventual non-smoothness of f when dividing the integration domain

7.2 Composite Quadrature

Definition 7.2.1 (Composite quadrature). Let $k \in \{2, 3, \dots\}$, let $-\infty < t_0 < t_1 < \dots < t_k < \infty$ and let Q_1 be a quadrature formula on $[t_0, t_1]$, let Q_2 be a quadrature formula on $[t_1, t_2], \dots$, let Q_k be a quadrature formula on $[t_{k-1}, t_k]$. Then a quadrature formula Q on $[t_0, t_k]$ is called **composite** (or: the **composition** of Q_1, \dots, Q_k) if

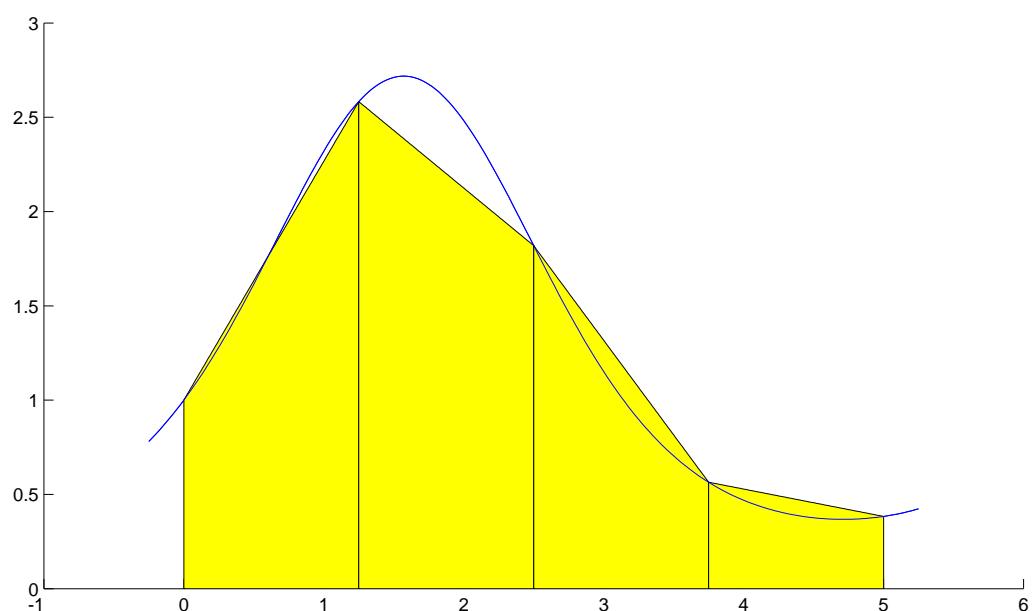
$$Q(f) = \sum_{j=1}^k Q_j(f|_{[t_{j-1}, t_j]}) \quad (7.2.1)$$

for all integrable functions $f: [t_0, t_k] \rightarrow \mathbb{R}$.

Example 7.2.1 (Simple composite quadrature formulas). Consider the setting of Definition 7.2.1 and let $a = t_0$ and $b = t_k$.

Composite trapezoidal rule:

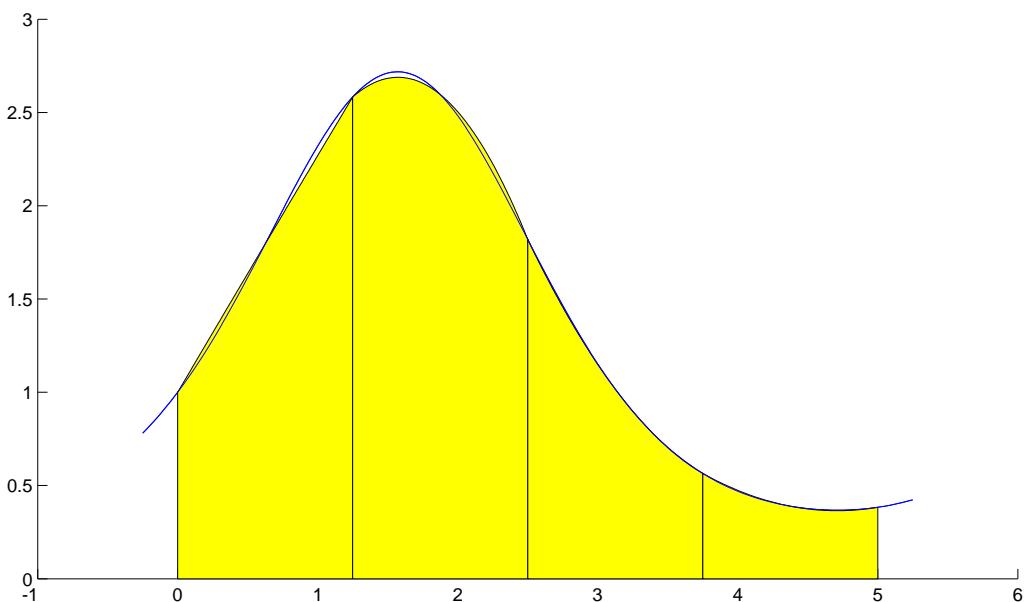
$$\int_a^b f(t)dt \approx \frac{1}{2}(t_1 - t_0)f(t_0) + \sum_{j=1}^{k-1} \frac{1}{2}(t_{j+1} - t_{j-1})f(t_j) + \frac{1}{2}(t_k - t_{k-1})f(t_k) \quad (7.2.3)$$
$$= Q_{t_0, t_1, \dots, t_{k-1}, t_k, [a, b]}^{\frac{t_1-t_0}{2}, \frac{t_2-t_0}{2}, \dots, \frac{t_k-t_{k-2}}{2}, \frac{t_k-t_{k-1}}{2}}(f)$$



Composite Simpson rule:

$$\int_a^b f(t) dt$$

$$\begin{aligned}
 &\approx \frac{1}{6}(t_1 - t_0)f(a) + \sum_{j=1}^{k-1} \frac{1}{6}(t_{j+1} - t_{j-1})f(t_j) + \sum_{j=1}^k \frac{2}{3}(t_j - t_{j-1})f\left(\frac{t_j+t_{j-1}}{2}\right) + \frac{1}{6}(t_k - t_{k-1})f(t_k) \\
 &= Q_{t_0, \frac{t_0+t_1}{2}, t_1, \frac{t_2+t_1}{2}, t_2, \dots, t_{k-1}, \frac{t_{k-1}+t_k}{2}, t_k, [a,b]}^{\frac{1}{6}(t_1-t_0), \frac{2}{3}(t_1-t_0), \frac{1}{6}(t_2-t_0), \frac{2}{3}(t_2-t_1), \frac{1}{6}(t_3-t_1), \dots, \frac{1}{6}(t_k-t_{k-2}), \frac{2}{3}(t_k-t_{k-1}), \frac{1}{6}(t_k-t_{k-1})}(f)
 \end{aligned} \tag{7.2.4}$$



Theorem 7.2.2 (Error analysis of composite quadrature formulas).

Let $-\infty < a < b < \infty$, $n, p \in \mathbb{N}$, $w_1, \dots, w_n \in \mathbb{R}$, $c_1, \dots, c_n \in [a, b]$ and let $\hat{Q} = Q_{c_1, \dots, c_n, [a, b]}^{w_1, \dots, w_n}$ be a quadrature formula of order p . Moreover, let $k \in \{2, 3, \dots\}$, let $-\infty < t_0 < t_1 < \dots < t_k < \infty$, let Q_1 be the transformation of \hat{Q} to $[t_0, t_1]$, ..., let Q_k be the transformation of \hat{Q} to $[t_{k-1}, t_k]$ (see Remark 7.1.1) and let Q be the **composition** of Q_1, \dots, Q_k . Then it holds for every $f \in C^p([t_0, t_k], \mathbb{R})$ that

$$\left| \int_{t_0}^{t_k} f(t) dt - Q(f) \right| \leq \left((t_k - t_0) \|f^{(p)}\|_{\infty, [t_0, t_k]} \left(1 + \frac{\sum_{j=1}^n |w_j|}{(b-a)} \right) \right) \left[\max_{1 \leq j \leq k} |t_j - t_{j-1}| \right]^p.$$

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Consider the setting of Theorem 7.2.2, let $\hat{a} = t_0$ and $\hat{b} = t_k$ and assume $h = t_j - t_{j-1}$ for all $j \in \{1, \dots, k\}$. Then we get from Theorem 7.2.2 that

$$\forall f \in C^p([\hat{a}, \hat{b}], \mathbb{R}): \quad E_Q(f) \leq \left((\hat{b} - \hat{a}) \|f^{(p)}\|_{\infty, [\hat{a}, \hat{b}]} \left(1 + \frac{\sum_{j=1}^n |w_j|}{(b-a)} \right) \right) h^p.$$

In particular, if \hat{Q} is the trapezoidal rule, then the **equidistant composite trapezoidal rule** satisfies

$$\forall f \in C^2([\hat{a}, \hat{b}], \mathbb{R}): \quad E_Q(f) \leq \left(2(\hat{b} - \hat{a}) \|f^{(2)}\|_{\infty, [\hat{a}, \hat{b}]} \right) h^2$$

and if \hat{Q} is the **Simpson rule**, then the equidistant composite Simpson rule satisfies

$$\forall f \in C^3([\hat{a}, \hat{b}], \mathbb{R}): \quad E_Q(f) \leq \left(2(\hat{b} - \hat{a}) \|f^{(3)}\|_{\infty, [\hat{a}, \hat{b}]} \right) h^3.$$

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