BASIC QUADRATURE METHODS

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David Levermore, 30 October 2016

1. Introduction. There are definite integrals that are either difficult or impossible to evaluate analytically. In such cases we can approximate the value of the integral by so-called **numerical integration** or **quadrature** methods. Most calculators and computers have routines that use such methods to approximately evaluate

$$\int_a^b f(x)\,dx$$

for any given integrand f and endpoints of integration a and b. The quadrature methods they use are advanced versions of the methods studied in elementary calculus courses, which we now review.

The quadrature methods studied in elementary calculus courses usually divide the interval $[a,b]$ into n uniform subintervals. The length Δx of each subinterval is given by

$$\Delta x \equiv \frac{b-a}{n}\,. \tag{1.1a}$$

The k^{th} subinterval is then $[x_{k-1}, x_k]$ where

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

with x_k given by the formula

$$x_k \equiv a + k\Delta x\,. \tag{1.1b}$$

Most basic quadrature methods associated with these subintervals are built from one or more Riemann sums of the form

$$\sum_{k=1}^{n} f(p_k)\,\Delta x\,, \quad \text{where } p_k \text{ is some point in } [x_{k-1}, x_k]. \tag{1.2}$$

When f is positive such a sum approximates the area under the curve $y = f(x)$ over the k^{th} subinterval by the area of a rectangle of height $f(p_k)$. Given an interval $[a,b]$ and a number of subintervals n, we compute Δx and the points x_k using (1.1). Then a Riemann sum in the form (1.2) for a given integrand f is determined by specifying a rule for choosing the points p_k.

The quadrature methods studied in most elementary calculus courses include three such Riemann sums.

- The so-called **left-hand rule** corresponds to the choice $p_k = x_{k-1}$, which is the left-hand endpoint of the k^{th} subinterval. When n uniform subintervals are used, we denote it by $\mathcal{Q}_n^L[f]$ and it is given by

$$\mathcal{Q}_n^L[f] = \sum_{k=1}^{n} f(x_{k-1})\,\Delta x\,. \tag{1.3}$$

- The so-called **right-hand rule** corresponds to the choice $p_k = x_k$, which is the right-hand endpoint of the k^{th} subinterval. When n uniform subintervals are used, we denote it by $\mathcal{Q}_n^R[f]$ and it is given by

$$\mathcal{Q}_n^R[f] = \sum_{k=1}^{n} f(x_k)\,\Delta x\,. \tag{1.4}$$

- The so-called **midpoint rule** corresponds to the choice $p_k = x_{k-\frac{1}{2}} \equiv \frac{1}{2}(x_{k-1} + x_k)$, which is the midpoint of the k^{th} subinterval. When n uniform subintervals are used, we denote it by $\mathcal{Q}_n^M[f]$ and it is given by

$$\mathcal{Q}_n^M[f] = \sum_{k=1}^{n} f(x_{k-\frac{1}{2}})\,\Delta x\,. \tag{1.5}$$

They also include two quadrature methods built from these Riemann sums.

- The **trapezoidal rule** is the average of the left-hand rule and the right-hand rule. When n uniform subintervals are used, we denote it by $\mathcal{Q}_n^T[f]$ and it is given by

$$\mathcal{Q}_n^T[f] = \tfrac{1}{2}\,\mathcal{Q}_n^L[f] + \tfrac{1}{2}\,\mathcal{Q}_n^R[f] = \sum_{k=1}^{n} \frac{f(x_{k-1}) + f(x_k)}{2}\,\Delta x\,. \tag{1.6}$$

- The **Simpson rule** is a weighted average of the left-hand rule, the right-hand rule, and the midpoint rule. When n uniform subintervals are used, we denote it by $\mathcal{Q}_n^S[f]$ and it is given by

$$\begin{aligned} \mathcal{Q}_n^S[f] &= \tfrac{1}{6}\,\mathcal{Q}_n^L[f] + \tfrac{2}{3}\,\mathcal{Q}_n^M[f] + \tfrac{1}{6}\,\mathcal{Q}_n^R[f] \\ &= \sum_{k=1}^{n} \frac{f(x_{k-1}) + 4f(x_{k-\frac{1}{2}}) + f(x_k)}{6}\,\Delta x\,. \end{aligned} \tag{1.7}$$

2. Left-Hand and Right-Hand Rules. The left-hand rule is given by (1.3) and the right-hand rule is given by (1.4). They are related by the identity

$$\mathcal{Q}_n^R[f] - \mathcal{Q}_n^L[f] = \big(f(b) - f(a)\big)\,\Delta x\,. \tag{2.1}$$

This identity should be evident both graphically and analytically.

The left-hand and right-hand rules are both clearly exact for constant functions. It is also clear both graphically and analytically that if f is increasing over $[a,b]$ then for every $x \in [x_{k-1}, x_k]$ we can bound $f(x)$ below and above as

$$f(x_{k-1}) \leq f(x) \leq f(x_k)\,.$$

Upon integrating these bounds over $[x_{k-1}, x_k]$ we obtain the inequalities

$$f(x_{k-1})\,\Delta x \leq \int_{x_{k-1}}^{x_k} f(x)\,dx \leq f(x_k)\,\Delta x\,.$$

By summing the above inequalities over $k = 1, \cdots, n$, we conclude that if f is increasing over $[a,b]$ then the left-hand rule gives an underestimate while the right-hand rule gives an overestimate:

$$\mathcal{Q}_n^L[f] \leq \int_a^b f(x)\,dx \leq \mathcal{Q}_n^R[f]\,. \tag{2.2a}$$

Similarly, if f is decreasing over $[a,b]$ then the right-hand rule gives an underestimate while the left-hand rule gives an overestimate:

$$\mathcal{Q}_n^R[f] \leq \int_a^b f(x)\,dx \leq \mathcal{Q}_n^L[f]\,. \tag{2.2b}$$

Hence, if f either is increasing over $[a,b]$ or is decreasing over $[a,b]$ then the right-hand and left-hand rules are each accurate to within $\big|\mathcal{Q}_n^R[f] - \mathcal{Q}_n^L[f]\big|$. However, by (2.1) we know that

$$\big|\mathcal{Q}_n^R[f] - \mathcal{Q}_n^L[f]\big| = |f(b) - f(a)|\,\Delta x\,.$$

Therefore, if f either is increasing over $[a,b]$ or is decreasing over $[a,b]$ then the error $\mathcal{E}_n[f]$ made by either the left-hand or right-hand rule satisfies

$$\big|\mathcal{E}_n[f]\big| \leq |f(b) - f(a)|\,\Delta x\,. \tag{2.3}$$

This upper bound for the size of the error can be made as small as we wish by picking n large enough. It decreases no slower than $1/n$ as n increases.

It will be shown in Section 5.1 that if f is any continuously differentiable function with $f(a) \neq f(b)$ then as $n \to \infty$ the leading order errors of $\mathcal{Q}_n^L[f]$ and $\mathcal{Q}_n^R[f]$ are given by

$$\begin{aligned} \mathcal{E}_n^L[f] &= \mathcal{Q}_n^L[f] - \int_a^b f(x)\,dx \sim -\tfrac{1}{2}\big(f(b)-f(a)\big)\,\Delta x\,, \\ \mathcal{E}_n^R[f] &= \mathcal{Q}_n^R[f] - \int_a^b f(x)\,dx \sim \tfrac{1}{2}\big(f(b)-f(a)\big)\,\Delta x\,. \end{aligned} \tag{2.4}$$

Notice that these errors have opposite signs, about equal magnitude, and decrease like $1/n$ as n increases. Moreover, they are consistent with (2.3).

3. Midpoint and Trapezoidal Rules. The midpoint rule is given by (1.5) and the trapezoidal rule is given by (1.6). The trapezoidal rule is the average of the left-hand and right-hand rules given by

$$\mathcal{Q}_n^T[f] = \tfrac{1}{2}\big(\mathcal{Q}_n^L[f] + \mathcal{Q}_n^R[f]\big)\,. \tag{3.1}$$

For this combination the leading order errors of $\mathcal{Q}_n^L[f]$ and $\mathcal{Q}_n^R[f]$ given by (2.4) cancel.

Both the midpoint and trapezoidal rules can be thought of as approximating the area under the curve over each subinterval by that of a trapezoid. In the case of the midpoint rule one side of the trapezoid is given by the tangent line at the midpoint of the subinterval, while in the case of the trapezoidal rule one side of the trapezoid is given by the secant line associated with the endpoints of the subinterval. Therefore the midpoint and trapezoidal rules are both exact for linear functions. This way of looking at these rules allows us to derive bounds on their errors when f either is convex over $[a,b]$ or is concave over $[a,b]$.

It should be clear graphically that if f is convex over $[a,b]$ then over each subinterval $[x_{k-1},x_k]$ the tangent line at the midpoint of the subinterval will lie below the graph of f while the secant line associated with the endpoints of the subinterval will lie above the graph of f. Expressed analytically, this states that for every $x \in [x_{k-1},x_k]$ we can bound $f(x)$ below and above by

$$f\big(x_{k-\frac{1}{2}}\big) + f'\big(x_{k-\frac{1}{2}}\big)\big(x - x_{k-\frac{1}{2}}\big) \leq f(x) \leq f(x_{k-1})\,\frac{x_k - x}{x_k - x_{k-1}} + f(x_k)\,\frac{x - x_{k-1}}{x_k - x_{k-1}}\,.$$

Upon integrating these bounds over $[x_{k-1},x_k]$ we obtain the inequalities

$$f\big(x_{k-\frac{1}{2}}\big)\,\Delta x \leq \int_{x_{k-1}}^{x_k} f(x)\,dx \leq \frac{f(x_{k-1}) + f(x_k)}{2}\,\Delta x\,,$$

where we have used the fact that $x_k - x_{k-1} = \Delta x$ and the facts that

$$\int_{x_{k-1}}^{x_k} \big(x - x_{k-\frac{1}{2}}\big)\,dx = 0\,, \qquad \int_{x_{k-1}}^{x_k} \frac{x_k - x}{x_k - x_{k-1}}\,dx = \int_{x_{k-1}}^{x_k} \frac{x - x_{k-1}}{x_k - x_{k-1}}\,dx = \frac{\Delta x}{2}\,.$$

By summing the above inequalities over $k = 1, \cdots, n$, we conclude that if f is convex over $[a, b]$ then the midpoint rule gives an underestimate while the trapezoidal rule gives an overestimate:

$$\mathcal{Q}_n^M[f] \leq \int_a^b f(x)\,dx \leq \mathcal{Q}_n^T[f]\,. \tag{3.2a}$$

Similarly, if f is concave over $[a, b]$ then the trapezoidal rule gives an underestimate while the midpoint rule gives an overestimate:

$$\mathcal{Q}_n^T[f] \leq \int_a^b f(x)\,dx \leq \mathcal{Q}_n^M[f]\,. \tag{3.2b}$$

Therefore if f either is convex over $[a, b]$ or is concave over $[a, b]$ then both the midpoint rule and the trapezoidal rule have errors no greater than $\big|\mathcal{Q}_n^T[f] - \mathcal{Q}_n^M[f]\big|$.

Next we show that the midpoint rule is always better than the trapezoidal rule when f either is convex over $[a, b]$ or is concave over $[a, b]$. The starting point is the fact that the midpoint and trapezoidal rules are related by

$$\mathcal{Q}_{2n}^T[f] = \tfrac{1}{2}\,\mathcal{Q}_n^T[f] + \tfrac{1}{2}\,\mathcal{Q}_n^M[f]\,. \tag{3.3}$$

If f is convex over $[a, b]$ then (3.2a) and (3.3) imply

$$\mathcal{Q}_n^M[f] \leq \int_a^b f(x)\,dx \leq \mathcal{Q}_{2n}^T[f] = \tfrac{1}{2}\,\mathcal{Q}_n^T[f] + \tfrac{1}{2}\,\mathcal{Q}_n^M[f]\,.$$

It follows that if f is convex over $[a, b]$ then

$$0 \leq \int_a^b f(x)\,dx - \mathcal{Q}_n^M[f] \leq \frac{\mathcal{Q}_n^T[f] - \mathcal{Q}_n^M[f]}{2} \leq \mathcal{Q}_n^T[f] - \int_a^b f(x)\,dx\,. \tag{3.4a}$$

Similarly, if f is concave over $[a, b]$ then

$$0 \leq \mathcal{Q}_n^M[f] - \int_a^b f(x)\,dx \leq \frac{\mathcal{Q}_n^M[f] - \mathcal{Q}_n^T[f]}{2} \leq \int_a^b f(x)\,dx - \mathcal{Q}_n^T[f]\,. \tag{3.4b}$$

Therefore, if f either is convex over $[a, b]$ or is concave over $[a, b]$ then the midpoint rule is better than the trapezoidal rule. This should also be evident graphically.

Remark. We see from (3.4) that if f either is convex over $[a, b]$ or is concave over $[a, b]$ then the midpoint rule error is not greater than $\frac{1}{2}\big|\mathcal{Q}_n^T[f] - \mathcal{Q}_n^M[f]\big|$, which improves upon our previous bound by a factor of $\frac{1}{2}$. In contrast, we see from (3.4) that the trapezoidal rule error is not smaller than $\frac{1}{2}\big|\mathcal{Q}_n^T[f] - \mathcal{Q}_n^M[f]\big|$.

Recall that when f either is increasing over $[a,b]$ or is decreasing over $[a,b]$ the size of the error made by either the left-hand or right-hand rule satisfies the upper bound given by (2.3). Similarly, there is an upper bound for the size of the error made by the midpoint and trapezoidal rules when f either is convex over $[a,b]$ or is concave over $[a,b]$. Because we have already shown that the midpoint rule is better than the trapezoidal rule in those cases, all that remains is to find an upper bound for the size of the error made by the trapezoidal rule.

We have seen from (3.2a) that when f is convex over $[a,b]$ the trapezoidal rule gives an overestimate for the integral over $[a,b]$. We now obtain an underestimate for the integral by replacing f with its tangent line approximation at x_k over each subinterval $[x_{k-\frac{1}{2}}, x_{k+\frac{1}{2}}]$. More specifically, for every $x \in [a, x_{\frac{1}{2}}]$ we bound $f(x)$ below by

$$f(a) + f'(a)(x-a) \leq f(x)\,, \tag{3.5a}$$

for every $k = 1, \cdots, n-1$ and every $x \in [x_{k-\frac{1}{2}}, x_{k+\frac{1}{2}}]$ we bound $f(x)$ below by

$$f(x_k) + f'(x_k)(x-x_k) \leq f(x)\,, \tag{3.5b}$$

and for every $x \in [x_{n-\frac{1}{2}}, b]$ we bound $f(x)$ below by

$$f(b) + f'(b)(x-b) \leq f(x)\,. \tag{3.5c}$$

Upon integrating bound (3.5a) for $f(x)$ over $[a, x_{\frac{1}{2}}]$, we obtain the inequality

$$f(a)\,\frac{\Delta x}{2} + f'(a)\,\frac{(\Delta x)^2}{8} \leq \int_a^{x_{\frac{1}{2}}} f(x)\,dx\,, \tag{3.6a}$$

where we have used the facts that

$$x_{\frac{1}{2}} - a = \frac{\Delta x}{2}\,, \qquad \int_a^{x_{\frac{1}{2}}} (x-a)\,dx = \frac{(\Delta x)^2}{8}\,.$$

Upon integrating bound (3.5b) for $f(x)$ over $[x_{k-\frac{1}{2}}, x_{k+\frac{1}{2}}]$, for every $k = 1, \cdots, n-1$ we obtain the inequality

$$f(x_k)\,\Delta x \leq \int_{x_{k-\frac{1}{2}}}^{x_{k+\frac{1}{2}}} f(x)\,dx\,, \tag{3.6b}$$

where we have used the facts that

$$x_{k+\frac{1}{2}} - x_{k-\frac{1}{2}} = \Delta x\,, \qquad \int_{x_{k-\frac{1}{2}}}^{x_{k+\frac{1}{2}}} (x-x_k)\,dx = 0\,.$$

Upon integrating bound (3.5c) for $f(x)$ over $[x_{n-\frac{1}{2}}, b]$, we obtain the inequality

$$f(b)\,\frac{\Delta x}{2} - f'(b)\,\frac{(\Delta x)^2}{8} \leq \int_{x_{n-\frac{1}{2}}}^{b} f(x)\,dx\,, \tag{3.6c}$$

where we have used the facts that

$$b - x_{n-\frac{1}{2}} = \frac{\Delta x}{2}\,, \qquad \int_{x_{n-\frac{1}{2}}}^{b} (x-b)\,dx = -\frac{(\Delta x)^2}{8}\,.$$

Remark. The fact that f is convex over $[a, b]$ implies that f' is increasing over $[a, b]$, whereby $f'(b) \geq f'(a)$ with equality if and only if f is linear over $[a, b]$.

By summing the inequalities (3.6), we see that if f is convex over $[a, b]$ then its integral over $[a, b]$ is underestimated by

$$\mathcal{Q}_n^T[f] - \tfrac{1}{8}\big(f'(b) - f'(a)\big)\,(\Delta x)^2 \leq \int_a^b f(x)\,dx\,.$$

By combining this underestimate with the fact from (3.2a) that $\mathcal{Q}_n^T[f]$ is an overestimate, we conclude that if f is convex over $[a, b]$ then

$$0 \leq \mathcal{Q}_n^T[f] - \int_a^b f(x)\,dx \leq \tfrac{1}{8}\big(f'(b) - f'(a)\big)\,(\Delta x)^2\,. \tag{3.7a}$$

Similarly, if f is concave over $[a, b]$ then

$$0 \leq \int_a^b f(x)\,dx - \mathcal{Q}_n^T[f] \leq -\tfrac{1}{8}\big(f'(b) - f'(a)\big)\,(\Delta x)^2\,. \tag{3.7b}$$

It follows from (3.4) and (3.7) that if f either is convex over $[a, b]$ or is concave over $[a, b]$ then the errors $\mathcal{E}_n^M[f]$ and $\mathcal{E}_n^T[f]$ made by the midpoint and trapezoidal rules satisfy

$$\big|\mathcal{E}_n^M[f]\big| \leq \big|\mathcal{E}_n^T[f]\big| \leq \tfrac{1}{8}\,|f'(b) - f'(a)|\,(\Delta x)^2\,. \tag{3.8}$$

This upper bound for the size of the error can be made as small as we wish by picking n large enough. It decreases no slower than n^{-2} as n increases. This is a much better rate of convergence than that given by (2.3) for the left-hand and right-hand rules.

It will be shown in Sections 5.2 and 5.3 that if f is any twice continuously differentiable function with $f'(a) \neq f'(b)$ then as $n \to \infty$ the leading order errors of $\mathcal{Q}_n^M[f]$ and $\mathcal{Q}_n^T[f]$ are given by

$$\mathcal{E}_n^M[f] = \mathcal{Q}_n^M[f] - \int_a^b f(x)\,dx \sim -\tfrac{1}{24}\big(f'(b) - f'(a)\big)\,(\Delta x)^2\,, \tag{3.9a}$$

$$\mathcal{E}_n^T[f] = \mathcal{Q}_n^T[f] - \int_a^b f(x)\,dx \sim \tfrac{1}{12}\big(f'(b) - f'(a)\big)\,(\Delta x)^2\,. \tag{3.9b}$$

Notice that the midpoint rule error is about half the size of the trapezoidal rule error. Moreover, they have opposite signs, decrease like n^{-2} as n increases, and are consistent with (3.8).

4. Simpson Rule. The Simpson rule is given by (1.7). It is the weighted average of the midpoint and trapezoidal rules given by

$$\mathcal{Q}_n^S[f] = \tfrac{2}{3}\,\mathcal{Q}_n^M[f] + \tfrac{1}{3}\,\mathcal{Q}_n^T[f]\,. \tag{4.1}$$

For this combination the leading order errors of $\mathcal{Q}_n^M[f]$ and $\mathcal{Q}_n^T[f]$ given by (3.9) cancel.

Remark. Because it follows from (3.3) that

$$\mathcal{Q}_n^M[f] = 2\mathcal{Q}_{2n}^T[f] - \mathcal{Q}_n^T[f]\,,$$

another way to think of the Simpson rule (4.1) is

$$\mathcal{Q}_n^S[f] = \tfrac{4}{3}\,\mathcal{Q}_{2n}^T - \tfrac{1}{3}\,\mathcal{Q}_n^T\,. \tag{4.2}$$

This is the way it will arise in the context of Romberg quadrature methods, which we will study later.

Because both the midpoint rule and the trapezoidal rule are exact for linear functions, it follows from (4.1) that the Simpson rule also is exact for linear functions. We now show that the Simpson rule is exact for cubic functions. To do this we must check that its error vanishes when f is a cubic function. We see from (1.8) that its error is given by

$$\begin{aligned}
\mathcal{E}_n^S[f] &= \mathcal{Q}_n^S[f] - \int_a^b f(x)\,dx \\
&= \sum_{k=1}^{n} \frac{f(x_{k-1}) + 4f(x_{k-\frac{1}{2}}) + f(x_k)}{6}\,\Delta x - \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} f(x)\,dx \\
&= \sum_{k=1}^{n} \left[\frac{f(x_{k-1}) + 4f(x_{k-\frac{1}{2}}) + f(x_k)}{6}\,\Delta x - \int_{x_{k-1}}^{x_k} f(x)\,dx \right].
\end{aligned}$$

For every k the quantity inside the square brackets is the error of the Simpson rule for the subinterval $[x_{k-1}, x_k]$. It is enough to show that for every k this quantity vanishes when f is a cubic function. Because every cubic function can be expressed as

$$f(x) = c_0 + c_1\big(x - x_{k-\frac{1}{2}}\big) + c_2\big(x - x_{k-\frac{1}{2}}\big)^2 + c_3\big(x - x_{k-\frac{1}{2}}\big)^3 ,$$

and because we already know that it vanishes for linear functions, we only have to check that it vanishes for

$$f(x) = \big(x - x_{k-\frac{1}{2}}\big)^2 \qquad \text{and} \qquad f(x) = \big(x - x_{k-\frac{1}{2}}\big)^3 .$$

For $f(x) = \big(x - x_{k-\frac{1}{2}}\big)^2$ we have

$$\begin{aligned} \frac{f(x_{k-1}) + 4f(x_{k-\frac{1}{2}}) + f(x_k)}{6}\,\Delta x &= \frac{\big(x_{k-1} - x_{k-\frac{1}{2}}\big)^2 + 4\cdot 0^2 + \big(x_k - x_{k-\frac{1}{2}}\big)^2}{6}\,\Delta x \\ &= \frac{\big(-\frac{1}{2}\Delta x\big)^2 + \big(\frac{1}{2}\Delta x\big)^2}{6}\,\Delta x = \frac{1}{24}\,(\Delta x)^3 , \end{aligned}$$

and

$$\begin{aligned} \int_{x_{k-1}}^{x_k} f(x)\,dx &= \int_{x_{k-1}}^{x_k} \big(x - x_{k-\frac{1}{2}}\big)^2\,dx = \frac{1}{3}\big(x - x_{k-\frac{1}{2}}\big)^3\Big|_{x_{k-1}}^{x_k} \\ &= \frac{\big(x_k - x_{k-\frac{1}{2}}\big)^3 - \big(x_{k-1} - x_{k-\frac{1}{2}}\big)^3}{3} = \frac{\big(\frac{1}{2}\Delta x\big)^3 - \big(-\frac{1}{2}\Delta x\big)^3}{3} = \frac{1}{24}\,(\Delta x)^3 . \end{aligned}$$

Because these are equal, the Simpson rule is exact for quadratic functions.

For $f(x) = \big(x - x_{k-\frac{1}{2}}\big)^3$ we can use the fact that $f(x)$ has odd symmetry about $x_{k-\frac{1}{2}}$ to conclude that

$$\frac{f(x_{k-1}) + 4f(x_{k-\frac{1}{2}}) + f(x_k)}{6}\,\Delta x = 0 ,$$

and that

$$\int_{x_{k-1}}^{x_k} f(x)\,dx = 0 .$$

Because these are equal, the Simpson rule is exact for cubic functions.

It will be shown in Section 5.4 that if f is any four times continuously differentiable function with $f'''(a) \neq f'''(b)$ then as $n \to \infty$ the leading order error of $\mathcal{Q}_n^S$ is given by

$$\mathcal{E}_n^S[f] = \mathcal{Q}_n^S[f] - \int_a^b f(x)\,dx \sim \tfrac{1}{2880}\,\big(f'''(b) - f'''(a)\big)\,(\Delta x)^4 . \tag{4.3}$$

Notice that the error of the Simpson rule decreases like n^{-4} as n increases.

5. Errors of Quadrature Methods. The error bounds given so far have required the integrand f to be either monotonic, convex, or concave over $[a, b]$. We now give expressions for the errors of these quadrature methods that allow error bounds to be derived for more general integrands. We will assume that f has as many continuous derivatives over $[a, b]$ as is needed for the calculations to make sense.

The first step is to find expressions for the error of each method for the case of only one subinterval ($n = 1$). These will just be summed to obtain expressions for the error when $n > 1$. The error for any Riemann sum with one term is

$$\mathcal{E}_1[f] = f(p)(b-a) - \int_a^b f(x)\,dx = \int_a^b [f(p) - f(x)]\,dx\,. \tag{5.1}$$

By the First Fundamental Theorem of Calculus

$$f(p) - f(x) = \int_x^p f'(y)\,dy\,.$$

This allows (5.1) to be expressed as

$$\begin{aligned}\mathcal{E}_1[f] = \int_a^b \int_x^p f'(y)\,dy\,dx &= \int_a^p \int_x^p f'(y)\,dy\,dx - \int_p^b \int_p^x f'(y)\,dy\,dx \\ &= \int_a^p \int_a^y f'(y)\,dx\,dy - \int_p^b \int_y^b f'(y)\,dx\,dy \\ &= \int_a^p (y-a) f'(y)\,dy - \int_p^b (b-y) f'(y)\,dy\,.\end{aligned} \tag{5.2}$$

5.1. Left-Hand and Right-Hand Rules. By setting $p = a$ in (5.2) we see that the error for the left-hand rule is

$$\mathcal{E}_1^L[f] = -\int_a^b (b-y) f'(y)\,dy\,. \tag{5.3a}$$

By setting $p = b$ in (5.2) we see that the error for the right-hand rule is

$$\mathcal{E}_1^R[f] = \int_a^b (y-a) f'(y)\,dy\,. \tag{5.3b}$$

All good estimates on the error of the left-hand and right-hand rules follow from (5.3a) and (5.3b) respectively. We will present several such estimates below. They are simpler versions of the analogous estimates for the other quadrature rules.

If $[a, b]$ is divided into n uniform subintervals $[x_{k-1}, x_k]$ as given by (1.1) then it follows from (5.3) that the errors of the left-hand and right-hand rules are

$$\mathcal{E}_n^L[f] = -\sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} (x_k - y) f'(y)\, dy\,, \tag{5.4a}$$

$$\mathcal{E}_n^R[f] = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} (y - x_{k-1}) f'(y)\, dy\,. \tag{5.4b}$$

If $|f'(y)| \leq M$ over $[a, b]$ then because

$$\int_{x_{k-1}}^{x_k} (x_k - y)\, dy = \int_{x_{k-1}}^{x_k} (y - x_{k-1})\, dy = \frac{(b-a)^2}{2\,n^2}\,,$$

we can obtain from (5.4) the bounds

$$\big|\mathcal{E}_n^L[f]\big| \leq \frac{(b-a)^2}{2\,n}\, M\,, \qquad \big|\mathcal{E}_n^R[f]\big| \leq \frac{(b-a)^2}{2\,n}\, M\,. \tag{5.5}$$

Alternatively, because

$$\max\big\{(x_k - y)\ :\ y \in [x_{k-1}, x_k]\big\} = \max\big\{(y - x_{k-1})\ :\ y \in [x_{k-1}, x_k]\big\} = \frac{b-a}{n}\,,$$

we can also obtain from (5.4) the bounds

$$\big|\mathcal{E}_n^L[f]\big| \leq \frac{b-a}{n} \int_a^b |f'(y)|\, dy\,, \qquad \big|\mathcal{E}_n^R[f]\big| \leq \frac{b-a}{n} \int_a^b |f'(y)|\, dy\,. \tag{5.6}$$

Both (5.5) and (5.6) show that these errors vanish at least as fast as n^{-1} as $n \to \infty$. Which bound is better depends upon f.

The bounds (5.6) reduce to the bound (2.3) that was derived earlier for the case when f is monotonic over $[a, b]$ because in that case

$$\int_a^b |f'(y)|\, dy = |f(b) - f(a)|\,.$$

Because the factors $(y - x_{k-1})$ and $(x_k - y)$ that appear inside the integrals in (5.4) are nonnegative, when f is monotonic over $[a, b]$ we can read off the sign of the errors given by (5.4). In particular, we recover the bounds (2.2).

Because the factors $(y - x_{k-1})$ and $(x_k - y)$ that appear inside the integrals in (5.4) are nonnegative, the Integral Mean-Value Theorem can be applied to conclude that

$$\int_{x_{k-1}}^{x_k} (x_k - y) f'(y)\, dy = \frac{(b-a)^2}{2\,n^2} f'(y_k^L) \qquad \text{for some } y_k^L \in [x_{k-1}, x_k]\,,$$
$$\int_{x_{k-1}}^{x_k} (y - x_{k-1}) f'(y)\, dy = \frac{(b-a)^2}{2\,n^2} f'(y_k^R) \qquad \text{for some } y_k^R \in [x_{k-1}, x_k]\,.$$

When these relations are placed into (5.4) it becomes

$$\mathcal{E}_n^L[f] = -\frac{b-a}{2\,n} \sum_{k=1}^{n} f'(y_k^L)\, \frac{b-a}{n} \quad \text{for some } y_k^L \in [x_{k-1}, x_k]\,, \tag{5.7a}$$
$$\mathcal{E}_n^R[f] = \frac{b-a}{2\,n} \sum_{k=1}^{n} f'(y_k^R)\, \frac{b-a}{n} \quad \text{for some } y_k^R \in [x_{k-1}, x_k]\,. \tag{5.7b}$$

Because the Intermediate-Value Theorem applied to f' yields

$$\frac{1}{n} \sum_{k=1}^{n} f'(y_k^L) = f'(y^L) \qquad \text{for some } y^L \in [a, b]\,,$$
$$\frac{1}{n} \sum_{k=1}^{n} f'(y_k^R) = f'(y^R) \qquad \text{for some } y^R \in [a, b]\,,$$

we see from (5.7) that

$$\mathcal{E}_n^L[f] = -\frac{(b-a)^2}{2\,n}\, f'(y^L) \qquad \text{for some } y^L \in [a, b]\,, \tag{5.8a}$$
$$\mathcal{E}_n^R[f] = \frac{(b-a)^2}{2\,n}\, f'(y^R) \qquad \text{for some } y^R \in [a, b]\,. \tag{5.8b}$$

These forms for the errors are often given in textbooks. We can derive (5.5) from them, but we cannot derive (5.6) from them.

Finally, because of the convergence of the Riemann sums

$$\lim_{n\to\infty} \sum_{k=1}^{n} f'(y_k^L)\,\frac{b-a}{n} = \int_a^b f'(y)\,dy = f(b) - f(a)\,,$$
$$\lim_{n\to\infty} \sum_{k=1}^{n} f'(y_k^R)\,\frac{b-a}{n} = \int_a^b f'(y)\,dy = f(b) - f(a)\,,$$

we see from (5.7) that if $f(b) \neq f(a)$ then

$$\mathcal{E}_n^L[f] \sim -\frac{b-a}{2\,n}\big(f(b) - f(a)\big) \qquad \text{as } n \to \infty\,, \tag{5.9a}$$
$$\mathcal{E}_n^R[f] \sim \frac{b-a}{2\,n}\big(f(b) - f(a)\big) \qquad \text{as } n \to \infty\,. \tag{5.9b}$$

These are the asymptotic convergence results that were asserted in (2.4). They show that the errors vanish like $1/n$ as $n \to \infty$ when $f(a) \neq f(b)$, and vanish faster when $f(a) = f(b)$.

Remark. It suffices to assume that f is continuously differentiable over $[a, b]$ to justify all the estimates above.

5.2. Midpoint Rule. The midpoint of $[a, b]$ is $c = \frac{1}{2}(a + b)$. By setting $p = c$ in (5.2) and integrating by parts we see that the error for the midpoint rule is

$$\begin{aligned}
\mathcal{E}_1^M[f] &= \int_a^c (y-a) f'(y)\,dy - \int_c^b (b-y) f'(y)\,dy \\
&= \tfrac{1}{2}(y-a)^2 f'(y)\Big|_a^c - \tfrac{1}{2}\int_a^c (y-a)^2 f''(y)\,dy \\
&\quad + \tfrac{1}{2}(b-y)^2 f'(y)\Big|_c^b - \tfrac{1}{2}\int_c^b (b-y)^2 f''(y)\,dy \\
&= -\tfrac{1}{2}\int_a^c (y-a)^2 f''(y)\,dy - \tfrac{1}{2}\int_c^b (b-y)^2 f''(y)\,dy\,.
\end{aligned} \tag{5.10}$$

Remark. Notice that the endpoint contributions from the integration by parts cancel. This canellation happened because we set $p = c$ in (5.2). It does not generally happen for any other value of p. This distinguishes the midpoint rule from all other Riemann sums.

If $[a,b]$ is divided into n uniform subintervals $[x_{k-1},x_k]$ as given by (1.1), each with midpoint $x_{k-\frac{1}{2}}$, then it follows from (5.10) that the error of the midpoint rule is

$$\mathcal{E}_n^M[f] = -\,\tfrac{1}{2}\sum_{k=1}^{n}\int_{x_{k-1}}^{x_{k-\frac{1}{2}}}(y-x_{k-1})^2 f''(y)\,dy - \tfrac{1}{2}\sum_{k=1}^{n}\int_{x_{k-\frac{1}{2}}}^{x_k}(x_k-y)^2 f''(y)\,dy\,. \tag{5.11}$$

If $|f''(y)|\leq M$ over $[a,b]$ then because

$$\int_{x_{k-1}}^{x_{k-\frac{1}{2}}}(y-x_{k-1})^2\,dy = \int_{x_{k-\frac{1}{2}}}^{x_k}(x_k-y)^2 f''(y)\,dy = \frac{(b-a)^3}{24\,n^3}\,,$$

we can obtain from (5.11) the bound

$$\big|\mathcal{E}_n^M[f]\big| \leq \frac{(b-a)^3}{24\,n^2}\,M\,. \tag{5.12}$$

Alternatively, because

$$\max\big\{(y-x_{k-1})^2\ :\ y\in[x_{k-1},x_{k-\frac{1}{2}}]\big\} = \max\big\{(x_k-y)^2\ :\ y\in[x_{k-\frac{1}{2}},x_k]\big\} = \frac{(b-a)^2}{4\,n^2}\,,$$

we can also obtain from (5.11) the bound

$$\big|\mathcal{E}_n^M[f]\big| \leq \frac{(b-a)^2}{8\,n^2}\int_a^b |f''(y)|\,dy\,. \tag{5.13}$$

Both (5.12) and (5.13) show that the error vanishes at least as fast as n^{-2} as $n\to\infty$. Which bound is better depends upon f.

Bound (5.13) reduces to the bound on $\mathcal{E}_n^M[f]$ in (3.8) that was derived earlier for the case when f is either convex or concave over $[a,b]$ because in that case

$$\int_a^b |f''(y)|\,dy = |f'(b)-f'(a)|\,.$$

Because the factors $(y-x_{k-1})^2$ and $(x_k-y)^2$ that appear inside the integrals in (5.11) are nonnegative, when f is either convex or concave over $[a,b]$ we can read off the sign of the error given by (5.11). In particular, we recover the bounds on $\mathcal{E}_n^M[f]$ given in (3.2).

Because the factors $(y-x_{k-1})^2$ and $(x_k-y)^2$ that appear inside the integrals in (5.11) are nonnegative, the Integral Mean-Value Theorem can be applied to conclude that

$$\begin{aligned}
\int_{x_{k-1}}^{x_{k-\frac{1}{2}}}(y-x_k)^2 f''(y)\,dy &= \frac{(b-a)^3}{24\,n^3}f''(y_k^-) \qquad \text{for some } y_k^-\in[x_{k-1},x_{k-\frac{1}{2}}]\,,\\
\int_{x_{k-\frac{1}{2}}}^{x_k}(x_k-y)^2 f''(y)\,dy &= \frac{(b-a)^3}{24\,n^3}f''(y_k^+) \qquad \text{for some } y_k^+\in[x_{k-\frac{1}{2}},x_k]\,.
\end{aligned}$$

When these relations are placed into (5.11) it becomes

$$\mathcal{E}_n^M[f] = -\frac{(b-a)^3}{24\,n^3} \sum_{k=1}^{n} \frac{f''(y_k^-) + f''(y_k^+)}{2} \qquad \text{for some } y_k^-, y_k^+ \in [x_{k-1}, x_k]\,. \tag{5.14}$$

Because the Intermediate-Value Theorem applied to f'' yields

$$\sum_{k=1}^{n} \frac{f''(y_k^-) + f''(y_k^+)}{2n} = f''(y^M) \qquad \text{for some } y^M \in [a,b]\,,$$

we see from (5.14) that

$$\mathcal{E}_n^M[f] = -\frac{(b-a)^3}{24\,n^2}\, f''(y^M) \qquad \text{for some } y^M \in [a,b]\,. \tag{5.15}$$

This form for the error is often given in textbooks. We can derive (5.12) from it, but we cannot derive (5.13) from it.

Finally, because of the convergence of the Riemann sums

$$\lim_{n\to\infty} \sum_{k=1}^{n} \frac{f''(y_k^-) + f''(y_k^+)}{2}\, \frac{b-a}{n} = \int_a^b f''(y)\, dy = f'(b) - f'(a)\,,$$

we see from (5.14) that if $f'(b) \neq f'(a)$ then

$$\mathcal{E}_n^M[f] \sim -\frac{(b-a)^2}{24\,n^2} \big(f'(b) - f'(a)\big) \qquad \text{as } n \to \infty\,, \tag{5.16}$$

This is the asymptotic convergence result that was asserted in (3.9a). It shows that the error vanishes like n^{-2} as $n \to \infty$ when $f'(a) \neq f'(b)$, and vanishes faster when $f'(a) = f'(b)$.

Remark. It suffices to assume that f is twice continuously differentiable over $[a,b]$ to justify all the estimates above.

5.3. Trapezoidal Rule. The trapezoidal rule is defined in terms of the left-hand and right-hand rules by (3.1). Because the errors of the left-hand and right-hand rules are given by (5.3), the error of the trapezoidal rule is

$$\begin{aligned}
\mathcal{E}_1^T[f] &= \tfrac{1}{2}\mathcal{E}_1^L[f] + \tfrac{1}{2}\mathcal{E}_1^R[f] \\
&= -\tfrac{1}{2}\int_a^b (b-y) f'(y)\, dy + \tfrac{1}{2}\int_a^b (y-a) f'(y)\, dy \\
&= -\tfrac{1}{2}\int_a^b \big((y-a)(b-y)\big)' f'(y)\, dy \\
&= -\tfrac{1}{2}\big((y-a)(b-y)\big) f'(y)\Big|_a^b + \tfrac{1}{2}\int_a^b (y-a)(b-y) f''(y)\, dy \\
&= \tfrac{1}{2}\int_a^b (y-a)(b-y) f''(y)\, dy\,.
\end{aligned} \tag{5.20}$$

Remark. Expression (5.20) is the starting point for the derivation of the Euler-Maclaurin formula, which lies at the heart of the Romberg quadrature methods we will study later.

If $[a,b]$ is divided into n uniform subintervals $[x_{k-1},x_k]$ as given by (1.1) then it follows from (5.20) that the error of the trapezoidal rule is

$$\mathcal{E}_n^T[f] = \tfrac{1}{2}\sum_{k=1}^{n}\int_{x_{k-1}}^{x_k}(y-x_{k-1})(x_k-y)f''(y)\,dy\,. \tag{5.21}$$

If $|f''(y)| \leq M$ over $[a,b]$ then because

$$\int_{x_{k-1}}^{x_k}(y-x_{k-1})(x_k-y)\,dy = \frac{(b-a)^3}{6\,n^3}\,,$$

we can obtain from (5.21) the bound

$$\big|\mathcal{E}_n^T[f]\big| \leq \frac{(b-a)^3}{12\,n^2}\,M\,. \tag{5.22}$$

Alternatively, because

$$\max\big\{(y-x_{k-1})(x_k-y)\,:\,y\in[x_{k-1},x_k]\big\} = \frac{(b-a)^2}{4\,n^2}\,,$$

we can also obtain from (5.21) the bound

$$\big|\mathcal{E}_n^T[f]\big| \leq \frac{(b-a)^2}{8\,n^2}\int_a^b|f''(y)|\,dy\,. \tag{5.23}$$

Both (5.22) and (5.23) show that the error vanishes at least as fast as n^{-2} as $n\to\infty$. Which bound is better depends upon f.

Bound (5.23) reduces to the bound on $\mathcal{E}_n^T[f]$ in (3.8) that was derived earlier for the case when f is either convex over $[a,b]$ or concave over $[a,b]$ because in that case

$$\int_a^b|f''(y)|\,dy = |f'(b)-f'(a)|\,.$$

Because the factor $(y-x_{k-1})(x_k-y)$ that appears inside the integral in (5.21) is nonnegative, when f is either convex or concave over $[a,b]$ we can read off the sign of the error given by (5.21). In particular, we recover the bounds on $\mathcal{Q}_n^T[f]$ given in (3.2).

Because the factor $(y - x_{k-1})(x_k - y)$ that appears inside the integral in (5.21) is nonnegative, the Integral Mean-Value Theorem can be applied to conclude that

$$\int_{x_{k-1}}^{x_k} (y - x_{k-1})(x_k - y) f''(y)\, dy = \frac{(b-a)^3}{12\, n^3}\, f''(y_k) \qquad \text{for some } y_k \in [x_{k-1}, x_k]\,.$$

When this relation is placed into (5.21) it becomes

$$\mathcal{E}_n^T[f] = \frac{(b-a)^3}{12\, n^3} \sum_{k=1}^{n} f''(y_k) \qquad \text{for some } y_k \in [x_{k-1}, x_k]\,. \tag{5.24}$$

Because the Intermediate-Value Theorem applied to f'' yields

$$\frac{1}{n} \sum_{k=1}^{n} f''(y_k) = f''(y^T) \qquad \text{for some } y^T \in [a, b]\,,$$

we see from (5.24) that

$$\mathcal{E}_n^T[f] = \frac{(b-a)^3}{12\, n^2}\, f''(y^T) \qquad \text{for some } y^T \in [a, b]\,. \tag{5.25}$$

This form for the error is often given in textbooks. We can derive (5.22) from it, but we cannot derive (5.23) from it.

Finally, because of the convergence of the Riemann sum

$$\lim_{n\to\infty} \sum_{k=1}^{n} f''(y_k)\, \frac{b-a}{n} = \int_a^b f''(y)\, dy = f'(b) - f'(a)\,,$$

we see from (5.24) that if $f'(b) \neq f'(a)$ then

$$\mathcal{E}_n^T[f] \sim \frac{(b-a)^2}{12\, n^2} \big(f'(b) - f'(a)\big) \qquad \text{as } n \to \infty\,, \tag{5.26}$$

This is the asymptotic convergence result that was asserted in (3.9b). It shows that the error vanishes like n^{-2} as $n \to \infty$ when $f'(a) \neq f'(b)$, and vanishes faster when $f'(a) = f'(b)$.

Remark. It suffices to assume that f is twice continuously differentiable over $[a, b]$ to justify all the estimates above.

5.4. Simpson Rule. The Simpson rule is defined in terms of the midpoint and trapezoidal rules by (4.1). Because the errors of the midpoint and trapezoidal rules are given by (5.10) and (5.20) respectively, after expressing the error as two integrals, some algebra in the integrands, and two integrations by parts for each integral, we see that the error of the Simpson rule is

$$\begin{aligned}
\mathcal{E}_1^S[f] &= \tfrac{2}{3}\mathcal{E}_1^M[f] + \tfrac{1}{3}\mathcal{E}_1^T[f] \\
&= -\tfrac{1}{3}\int_a^c (y-a)^2 f''(y)\,dy - \tfrac{1}{3}\int_c^b (b-y)^2 f''(y)\,dy \\
&\quad + \tfrac{1}{6}\int_a^b (y-a)(b-y) f''(y)\,dy \\
&= \tfrac{1}{6}\int_a^c \big((y-a)(b-y) - 2(y-a)^2\big) f''(y)\,dy \\
&\quad + \tfrac{1}{6}\int_c^b \big((y-a)(b-y) - 2(b-y)^2\big) f''(y)\,dy \\
&= \tfrac{1}{6}\int_a^c \big(2(y-a)(c-y) - (y-a)^2\big) f''(y)\,dy \\
&\quad + \tfrac{1}{6}\int_c^b \big(2(y-c)(b-y) - (b-y)^2\big) f''(y)\,dy \\
&= \tfrac{1}{6}\int_a^c (y-a)^2(c-y) f'''(y)\,dy \\
&\quad - \tfrac{1}{6}\int_c^b (y-c)(b-y)^2 f'''(y)\,dy \\
&= \tfrac{1}{18}\int_a^c \big[(y-a)^3(c-y) + \tfrac{1}{4}(y-a)^4\big] f^{(4)}(y)\,dy \\
&\quad + \tfrac{1}{18}\int_c^b \big[(y-c)(b-y)^3 + \tfrac{1}{4}(b-y)^4\big] f^{(4)}(y)\,dy\,.
\end{aligned} \tag{5.30}$$

In what follows we will make use of the facts that

$$\begin{aligned}
0 \le (y-a)^3(c-y) + \tfrac{1}{4}(y-a)^4 &\le \tfrac{1}{4}(c-a)^4 = \tfrac{1}{64}(b-a)^4 \qquad \text{over } [a,c]\,, \\
0 \le (y-c)(b-y)^3 + \tfrac{1}{4}(b-y)^4 &\le \tfrac{1}{4}(b-c)^4 = \tfrac{1}{64}(b-a)^4 \qquad \text{over } [c,b]\,,
\end{aligned} \tag{5.31}$$

and that

$$\begin{aligned}
\int_a^c \big[(y-a)^3(c-y) + \tfrac{1}{4}(y-a)^4\big]\,dy &= \tfrac{1}{10}(c-a)^5 = \tfrac{1}{320}(b-a)^5\,, \\
\int_c^b \big[(y-c)(b-y)^3 + \tfrac{1}{4}(b-y)^4\big]\,dy &= \tfrac{1}{10}(b-c)^5 = \tfrac{1}{320}(b-a)^5\,.
\end{aligned} \tag{5.32}$$

If $[a, b]$ is divided into n uniform subintervals $[x_{k-1}, x_k]$ as given by (1.1) then it follows from (5.30) that the error of the Simpson rule is

$$\begin{aligned}\mathcal{E}_n^S[f] &= \tfrac{1}{18}\sum_{k=1}^{n}\int_{x_{k-1}}^{x_{k-\frac12}} \left[(y-x_{k-1})^3(x_{k-\frac12}-y)-\tfrac14(y-x_{k-1})^4\right] f^{(4)}(y)\,dy \\ &\quad + \tfrac{1}{18}\sum_{k=1}^{n}\int_{x_{k-\frac12}}^{x_k} \left[(y-x_{k-\frac12})(x_k-y)^3+\tfrac14(x_k-y)^4\right] f^{(4)}(y)\,dy\,.\end{aligned} \tag{5.33}$$

If $|f^{(4)}(y)| \leq M$ over $[a, b]$ then because by (5.32)

$$\int_{x_{k-1}}^{x_{k-\frac12}} \left[(y-x_{k-1})^3(x_{k-\frac12}-y)-\tfrac14(y-x_{k-1})^4\right] dy = \frac{(b-a)^5}{320\,n^5}\,,$$

$$\int_{x_{k-\frac12}}^{x_k} \left[(y-x_{k-\frac12})(x_k-y)^3+\tfrac14(x_k-y)^4\right] dy = \frac{(b-a)^5}{320\,n^5}\,,$$

we can obtain from (5.33) the bound

$$\left|\mathcal{E}_n^S[f]\right| \leq \frac{(b-a)^5}{2880\,n^4}\,M\,. \tag{5.34}$$

Alternatively, because by (5.31)

$$\max\left\{(y-x_{k-1})^3(x_{k-\frac12}-y)-\tfrac14(y-x_{k-1})^4 \,:\, y\in[x_{k-1},x_{k-\frac12}]\right\} = \frac{(b-a)^4}{64\,n^4}\,,$$

$$\max\left\{(y-x_{k-\frac12})(x_k-y)^3+\tfrac14(x_k-y)^4 \,:\, y\in[x_{k-\frac12},x_k]\right\} = \frac{(b-a)^4}{64\,n^4}\,,$$

we can also obtain from (5.33) the bound

$$\left|\mathcal{E}_n^S[f]\right| \leq \frac{(b-a)^4}{1152\,n^4}\int_a^b |f^{(4)}(y)|\,dy\,. \tag{5.35}$$

Both (5.34) and (5.35) show that the error vanishes at least as fast as n^{-4} as $n \to \infty$. Which bound is better depends upon f.

When f''' is monotonic over $[a, b]$ then

$$\int_a^b |f^{(4)}(y)|\,dy = |f'''(b)-f'''(a)|\,,$$

in which case (5.35) can be recast as

$$\left|\mathcal{E}_n^S[f]\right| \leq \frac{(b-a)^4}{1152\,n^4}\,|f'''(b)-f'''(a)|\,. \tag{5.36}$$

Because the factors inside the square brackets of the integrands in (5.33) are nonnegative, when f''' is monotonic over $[a,b]$ we can read off the sign of the error given by (5.33).

Because the factors that appear inside the square brackets of the integrands in (5.33) are nonnegative, the Integral Mean-Value Theorem can be applied to conclude that

$$\int_{x_{k-1}}^{x_{k-\frac{1}{2}}} \left[(y-x_{k-1})^3(x_{k-\frac{1}{2}}-y) - \tfrac{1}{4}(y-x_{k-1})^4\right] f^{(4)}(y)\,dy = \frac{(b-a)^5}{5760\,n^5} f^{(4)}(y_k^-) \qquad \text{for some } y_k^- \in [x_{k-1}, x_{k-\frac{1}{2}}]\,,$$

$$\int_{x_{k-\frac{1}{2}}}^{x_k} \left[(y-x_{k-\frac{1}{2}})(x_k-y)^3 + \tfrac{1}{4}(x_k-y)^4\right] f^{(4)}(y)\,dy = \frac{(b-a)^5}{5760\,n^5} f^{(4)}(y_k^+) \qquad \text{for some } y_k^+ \in [x_{k-\frac{1}{2}}, x_k]\,.$$

When these relations are placed into (5.33) it becomes

$$\mathcal{E}_n^S[f] = \frac{(b-a)^5}{2880\,n^5} \sum_{k=1}^{n} \frac{f^{(4)}(y_k^-) + f^{(4)}(y_k^+)}{2} \qquad \text{for some } y_k^-, y_k^+ \in [x_{k-1}, x_k]\,. \tag{5.37}$$

Because the Intermediate-Value Theorem applied to $f^{(4)}$ yields

$$\sum_{k=1}^{n} \frac{f^{(4)}(y_k^-) + f^{(4)}(y_k^+)}{2n} = f''(y^S) \qquad \text{for some } y^S \in [a,b]\,,$$

we see from (5.35) that

$$\mathcal{E}_n^S[f] = -\frac{(b-a)^5}{2880\,n^4} f^{(4)}(y^S) \qquad \text{for some } y^S \in [a,b]\,. \tag{5.38}$$

This form for the error is equivalent to one often given in textbooks. We can derive (5.34) from it, but we cannot derive (5.35) from it.

Finally, because of the convergence of the Riemann sums

$$\lim_{n\to\infty} \sum_{k=1}^{n} \frac{f^{(4)}(y_k^-) + f^{(4)}(y_k^+)}{2} \, \frac{b-a}{n} = \int_a^b f^{(4)}(y)\,dy = f'''(b) - f'''(a)\,,$$

we see from (5.37) that if $f'''(b) \neq f'''(a)$ then

$$\mathcal{E}_n^S[f] \sim -\frac{(b-a)^4}{2880\,n^4} \big(f'''(b) - f'''(a)\big) \qquad \text{as } n \to \infty\,, \tag{5.39}$$

This is the asymptotic convergence result that was asserted in (4.3). It shows that the error vanishes like n^{-4} as $n \to \infty$ when $f'''(a) \neq f'''(b)$, and vanishes faster when $f'''(a) = f'''(b)$.

Remark. It suffices to assume that f is four times continuously differentiable over $[a,b]$ to justify all the estimates above.