CSER 2207: Numerical Analysis

Lecture-14
Numerical Integration

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Elements of Numerical Integration

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain. The basic method involved in approximating $\int_a^b f(x)\,dx$ is called **numerical quadrature**. It uses a sum $\sum_{i=0}^{n} a_i f(x_i)$ to approximate $\int_a^b f(x)\,dx$.

The methods of quadrature in this section are based on the interpolation polynomials given in Chapter 3. The basic idea is to select a set of distinct nodes $\{x_0, \ldots, x_n\}$ from the interval $[a, b]$. Then integrate the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x)$$

and its truncation error term over $[a, b]$ to obtain

$$\int_a^b f(x)\,dx = \int_a^b \sum_{i=0}^{n} f(x_i) L_i(x)\,dx + \int_a^b \prod_{i=0}^{n} (x - x_i) \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,dx$$

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$$= \sum_{i=0}^{n} a_i f(x_i) + \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i) f^{(n+1)}(\xi(x))\, dx,$$

where $\xi(x)$ is in $[a, b]$ for each x and

$$a_i = \int_a^b L_i(x)\, dx, \quad \text{for each } i = 0, 1, \ldots, n.$$

The quadrature formula is, therefore,

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

with error given by

$$E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i) f^{(n+1)}(\xi(x))\, dx.$$

Before discussing the general situation of quadrature formulas, let us consider formulas produced by using first and second Lagrange polynomials with equally-spaced nodes. This gives the **Trapezoidal rule** and **Simpson's rule**, which are commonly introduced in calculus courses.

Trapezoidal Rule

To derive the Trapezoidal rule for approximating $\int_a^b f(x)\,dx$, let $x_0 = a$, $x_1 = b$, $h = b - a$ and use the linear Lagrange polynomial:

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1).$$

Then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] dx + \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\,dx. \tag{4.23}$$

The product $(x - x_0)(x - x_1)$ does not change sign on $[x_0, x_1]$, so the Weighted Mean Value Theorem for Integrals 1.13 can be applied to the error term to give, for some ξ in (x_0, x_1),

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$$\begin{aligned}\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)\,dx &= f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx\\ &= f''(\xi)\left[\frac{x^3}{3}-\frac{(x_1+x_0)}{2}x^2+x_0x_1x\right]_{x_0}^{x_1}\\ &= -\frac{h^3}{6}f''(\xi).\end{aligned}$$

Consequently, Eq. (4.23) implies that

$$\begin{aligned}\int_a^b f(x)\,dx &= \left[\frac{(x-x_1)^2}{2(x_0-x_1)}f(x_0)+\frac{(x-x_0)^2}{2(x_1-x_0)}f(x_1)\right]_{x_0}^{x_1}-\frac{h^3}{12}f''(\xi)\\ &= \frac{(x_1-x_0)}{2}[f(x_0)+f(x_1)]-\frac{h^3}{12}f''(\xi).\end{aligned}$$

Using the notation $h = x_1 - x_0$ gives the following rule:

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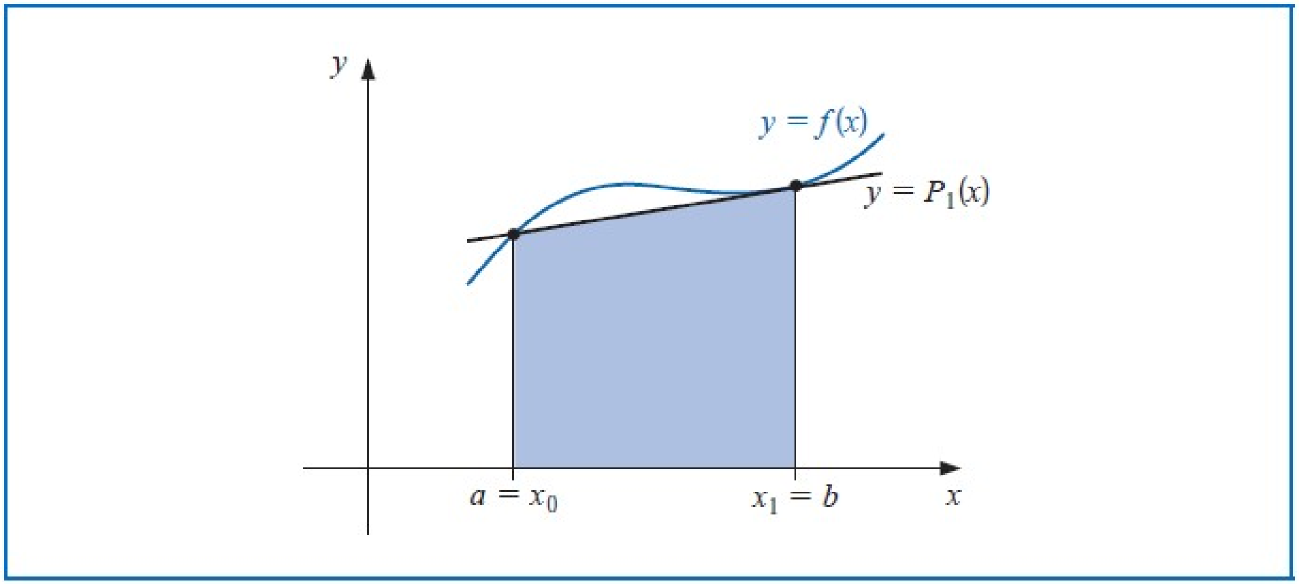
Trapezoidal Rule:

$$\int_a^b f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi).$$

This is called the Trapezoidal rule because when f is a function with positive values, $\int_a^b f(x)\,dx$ is approximated by the area in a trapezoid, as shown in Figure 4.3.

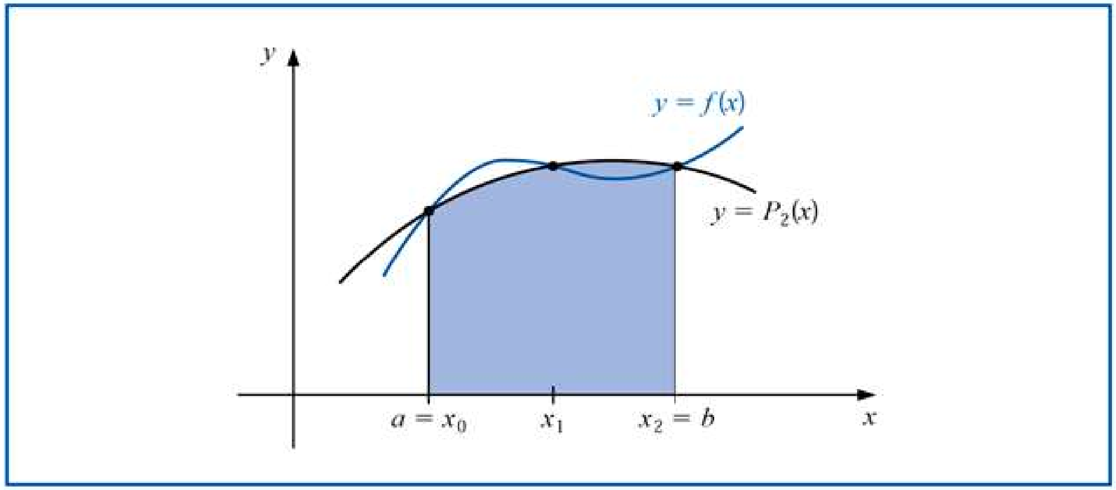
Figure 4.3



Simpson's Rule

Simpson's rule results from integrating over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a$, $x_2 = b$, and $x_1 = a + h$, where $h = (b - a)/2$. (See Figure 4.4.)

Figure 4.4



Therefore

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} \left[\frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \right] dx + \int_{x_0}^{x_2} \frac{(x - x_0)(x - x_1)(x - x_2)}{6} f^{(3)}(\xi(x))\,dx.$$

Cont…

Deriving Simpson's rule in this manner, however, provides only an $O(h^4)$ error term involving $f^{(3)}$. By approaching the problem in another way, a higher-order term involving $f^{(4)}$ can be derived.

To illustrate this alternative method, suppose that f is expanded in the third Taylor polynomial about x_1. Then for each x in $[x_0, x_2]$, a number $\xi(x)$ in (x_0, x_2) exists with

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f'''(x_1)}{6}(x - x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x - x_1)^4$$

and

$$\int_{x_0}^{x_2} f(x)\,dx = \left[f(x_1)(x - x_1) + \frac{f'(x_1)}{2}(x - x_1)^2 + \frac{f''(x_1)}{6}(x - x_1)^3 + \frac{f'''(x_1)}{24}(x - x_1)^4 \right]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4\,dx. \quad (4.24)$$

Because $(x - x_1)^4$ is never negative on $[x_0, x_2]$, the Weighted Mean Value Theorem for Integrals 1.13 implies that

$$\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x - x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{120}(x - x_1)^5\Big]_{x_0}^{x_2},$$

for some number ξ_1 in (x_0, x_2).

However, $h = x_2 - x_1 = x_1 - x_0$, so

$$(x_2 - x_1)^2 - (x_0 - x_1)^2 = (x_2 - x_1)^4 - (x_0 - x_1)^4 = 0,$$

whereas

$$(x_2 - x_1)^3 - (x_0 - x_1)^3 = 2h^3 \quad \text{and} \quad (x_2 - x_1)^5 - (x_0 - x_1)^5 = 2h^5.$$

Consequently, Eq. (4.24) can be rewritten as

$$\int_{x_0}^{x_2} f(x)\,dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{60}h^5.$$

If we now replace $f''(x_1)$ by the approximation given in Eq. (4.9) of Section 4.1, we have

$$\int_{x_0}^{x_2} f(x)\,dx = 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2)\right\} + \frac{f^{(4)}(\xi_1)}{60}h^5$$
$$= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12}\left[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\right].$$

It can be shown by alternative methods (see Exercise 24) that the values ξ_1 and ξ_2 in this expression can be replaced by a common value ξ in (x_0, x_2). This gives Simpson's rule.

Example

Simpson's Rule:

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi).$$

The error term in Simpson's rule involves the fourth derivative of f, so it gives exact results when applied to any polynomial of degree three or less.

Example 1 Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)\,dx$ when $f(x)$ is

(a)	x^2	**(b)**	x^4	**(c)**	$(x+1)^{-1}$
(d)	$\sqrt{1+x^2}$	**(e)**	$\sin x$	**(f)**	e^x

Solution On $[0, 2]$ the Trapezoidal and Simpson's rule have the forms

$$\text{Trapezoid:} \quad \int_0^2 f(x)\,dx \approx f(0) + f(2) \quad \text{and}$$

$$\text{Simpson's:} \quad \int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

Cont...

The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^2$.

The results to three places for the functions are summarized in Table 4.7. Notice that in each instance Simpson's Rule is significantly superior. ■

Table 4.7

	(a)	(b)	(c)	(d)	(e)	(f)
$f(x)$	x^2	x^4	$(x+1)^{-1}$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

Thank You