Lecture 5: Numerical quadratures

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Since polynomials are easy to integrate, the idea, roughly speaking, is to approximate the function f by its Lagrange interpolation polynomial p_n of degree n, and integrate p_n instead. Thus,

$$\int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx \tag{1}$$

Newton-Cotes formulae

For a positive integer n, let $x_i, i = 0, \ldots, n$, denote the interpolation points; for the sake of simplicity, we shall assume that these are equally spaced, namely,

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$$w_k = \int_a^b L_k(x)\,dx, \quad k = 0, \ldots, n$$

Definition

Numerical quadrature rules, with equally spaced quadrature points, are called Newton-Cotes formulae.

In order to illustrate the general idea, we consider two simple examples:

- Trapezium rule.
- Simpson's rule.

Trapezium rule

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p_1(x) &= L_0(x)f(x_0) + L_1(x)f(x_1) \\
&= \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \\
&= \frac{1}{b - a}[(b - x)f(a) + (x - a)f(b)]
\end{aligned}
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Integrating $p_1(x)$ from a to b yields

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Integrating $p_1(x)$ from a to b yields

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This numerical integration formula is called the trapezium rule.

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$$x_0 = a, x_1 = (a+b)/2 \text{ and } x_2 = b$$

the Lagrange polynomial of degree 2, with these interpolation points, for the function f is:

$$\begin{aligned}
p_2(x) &= L_0(x)f(x_0) + L_1(x)f(x_1) + L_2(x)f(x_2) \\
&= \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).
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Integrating $p_2(x)$ from a to b gives

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

This numerical integration formula is known as Simpson's rule.

Error estimate

Our next task is to estimate the size of the error in the numerical integration formula (2), that is, the error that has been committed by integrating the Lagrange interpolation polynomial of f instead of the function f itself.

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$$E_n(f) = \int_a^b f(x)\,dx - \sum_{k=0}^{n} w_k f(x_k)$$

The next theorem provides a useful bound on $E_n(f)$ under the additional hypothesis that the function f is sufficiently smooth.

Theorem 1

Suppose that f is a real-valued function defined on the interval $[a, b]$, and let $f^{(n+1)}$ be continuous on $[a, b]$. Then,

$$|E_n(f)| \leq \frac{M_{n+1}}{(n+1)!} \int_a^b |\pi_{n+1}(x)| \, dx \tag{3}$$

where :

- $M_{n+1} = \max_{\zeta \in [a,b]} \left| f^{(n+1)}(\zeta) \right|$ and
- $\pi_{n+1}(x) = (x - x_0) \ldots (x - x_n)$.

Proof:

Recalling the inequality:

$$|f(x) - p_n(x)| \leq \frac{M_{n+1}}{(n+1)!} |\pi_{n+1}(x)| \tag{4}$$

and the definition of the weights w_k in (2),

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and the definition of the weights w_k in (2), we can rewrite $E_n(f)$ as follows:

$$\begin{aligned} E_n(f) &= \int_a^b f(x)\,dx - \int_a^b \left(\sum_{k=0}^{n} L_k(x) f\left(x_k\right) \right) dx \\ &= \int_a^b \left(f(x) - p_n(x) \right) dx \end{aligned}$$

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Thus,

$$|E_n(f)| \leq \int_a^b |f(x) - p_n(x)|\, dx$$

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Thus,

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The desired error estimate (3) follows by inserting (4) into the right-hand side of this inequality.

Let us apply Theorem 1 to estimate the size of the error that has been committed by applying the trapezium rule to the integral $\int_a^b f(x)\,dx$. In this case (3) reduces to

$$
\begin{aligned}
|E_1(f)| &\leq \frac{1}{2} M_2 \int_a^b |(x-a)(x-b)|\,dx \\
&= \frac{1}{2} M_2 \int_a^b (b-x)(x-a)\,dx \\
&= \frac{1}{12} (b-a)^3 M_2 \qquad (14)
\end{aligned}
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An analogous but slightly more tedious calculation shows that, for Simpson's rule,

$$
\begin{aligned}
|E_2(f)| &\leq \frac{1}{6} M_3 \int_a^b \left|(x-a)\left(x-\frac{a+b}{2}\right)(x-b)\right|\,dx \qquad (5) \\
&= \frac{1}{192} M_3 (b-a)^4 \qquad (6)
\end{aligned}
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Lemma 1

Suppose that f is a real-valued function defined on the interval $[a, b]$ and $f^{(4)}$ is a continuous function on $[a, b]$. Then

$$\int_a^b f(x)dx - \frac{b-a}{6}\left[f(a) + f\left(\frac{a+b}{2}\right) + f(b)\right] = -\frac{(b-a)^5}{2880} f^{(4)}(\xi) \quad (7)$$

for some ξ in (a, b).

Proof:

Performing the change of variables

$$x = \frac{a+b}{2} + \frac{b-a}{2}t, \quad t \in [-1, 1]$$

and defining the function $t \mapsto F(t)$ by $F(t) = f(x)$, we have that

$$\int_a^b f(x)\,dx - \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \tag{8}$$

$$= \frac{b-a}{2}\left(\int_{-1}^{1} F(t)\,dt - \frac{1}{3}[F(-1) + 4F(0) + F(1)]\right) \tag{9}$$

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$$G(t) = \int_{-t}^{t} F(\tau)\mathrm{d}\tau - \frac{t}{3}[F(-t) + 4F(0) + F(t)], \quad t \in [-1, 1]$$

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Now

$$G^{(4)}(t) = -\frac{1}{3}\left(F'''(t) - F'''(-t)\right) - \frac{t}{3}\left(F^{(4)}(t) + F^{(4)}(-t)\right)$$

and therefore

$$G(1) = -\frac{1}{360\zeta_4}\left(F'''(\zeta_4) - F'''(-\zeta_4)\right) - \frac{1}{360}\left(F^{(4)}(\zeta_4) + F^{(4)}(-\zeta_4)\right)$$

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Applying Lagrange's Mean Value Theorem to the first term on the right, we deduce that

$$G(1) = -\frac{1}{180}F^{(4)}(\zeta_5) - \frac{1}{360}\left(F^{(4)}(\zeta_4) + F^{(4)}(-\zeta_4)\right)$$

for some $\zeta_5 \in (-\zeta_4, \zeta_4)$.

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for some $\zeta_5 \in (-\zeta_4, \zeta_4)$.Equivalently, Since, by our hypothesis on $f, F^{(4)}$ is a continuous function on $[-1,1]$ and $-1 < -\zeta_4 < \zeta_5 < \zeta_4 < 1$, it follows that there exists θ in $[-\zeta_4, \zeta_4]$ such that

$$\frac{F^{(4)}\left(-\zeta_4\right) + 2F^{(4)}\left(\zeta_5\right) + F^{(4)}\left(\zeta_4\right)}{4} = F^{(4)}(\theta)$$

consequently,

$$G(1) = -\frac{1}{90}F^{(4)}(\theta) = -\frac{1}{1440}(b-a)^4 f^{(4)}(\xi) \tag{10}$$

where $\xi = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)\theta$.

Since, by our hypothesis on f, $F^{(4)}$ is a continuous function on $[-1, 1]$ and $-1 < -\zeta_4 < \zeta_5 < \zeta_4 < 1$, it follows that there exists θ in $[-\zeta_4, \zeta_4]$ such that

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where $\xi = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)\theta$.Finally, (7) is obtained by inserting (10) into (9).

Now Lemma 1 yields the following bound on the error in Simpson's rule:

$$|E_2(f)| \le \frac{1}{2880}(b-a)^5 M_4 \tag{11}$$

Since, by our hypothesis on f, $F^{(4)}$ is a continuous function on $[-1,1]$ and $-1 < -\zeta_4 < \zeta_5 < \zeta_4 < 1$, it follows that there exists θ in $[-\zeta_4, \zeta_4]$ such that

$$\frac{F^{(4)}(-\zeta_4) + 2F^{(4)}(\zeta_5) + F^{(4)}(\zeta_4)}{4} = F^{(4)}(\theta)$$

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This is a considerable improvement over (5) in the sense that if $f \in \mathcal{P}_3$ then the right-hand side of (11) is equal to zero and thereby $E_2(f) = 0$ which now correctly reflects the fact that polynomials of degree three are integrated by Simpson's rule

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without error. (As remarked earlier, this property was not borne out by our initial crude bound (5).)

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Composite trapezium rule

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This is obtained by dividing the interval $[a, b]$ into m equal subintervals, each of width $h = (b - a)/m$, so that

$$\int_a^b f(x)\, dx = \sum_{i=1}^{m} \int_{x_{i-1}}^{x_i} f(x)\, dx$$

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Each of the integrals is then evaluated by the trapezium rule, namely,

$$\int_{x_{i-1}}^{x_i} f(x)\, dx \approx \frac{1}{2} h \left[f\left(x_{i-1}\right) + f\left(x_i\right)\right]$$

giving the complete approximation

$$\int_a^b f(x)\, dx \approx h\left[\frac{1}{2} f\left(x_0\right) + f\left(x_1\right) + \ldots + f\left(x_{m-1}\right) + \frac{1}{2} f\left(x_m\right)\right] \tag{12}$$

Error in composite rules

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The error in the composite trapezium rule can be estimated by using the error bound (**??**) for the trapezium rule on each individual subinterval $[x_{i-1}, x_i]$, $i = 1, \ldots, m$.Indeed,

$$\mathcal{E}_1(f) := \int_a^b f(x)\,dx - h\left[\frac{1}{2}f(x_0) + f(x_1) + \ldots + f(x_{m-1}) + \frac{1}{2}f(x_m)\right]$$
$$= \sum_{i=1}^{m}\left[\int_{x_{i-1}}^{x_i} f(x)\,dx - \frac{1}{2}h\left[f(x_{i-1}) + f(x_i)\right]\right]$$

Applying (**??**) to each of the terms under the summation sign,

$$|\mathcal{E}_1(f)| \leq \frac{1}{12}h^3\sum_{i=1}^{m}\left(\max_{\zeta\in[x_{i-1},x_i]}|f''(\zeta)|\right) \tag{13}$$
$$\leq \frac{1}{12m^2}(b-a)^3 M_2, \tag{14}$$

where $M_2 = \max_{\zeta\in[a,b]}|f''(\zeta)|$.

Composite Simpson's rule.

Let us suppose that the interval $[a, b]$ has been divided into $2m$ subintervals by the points $x_i = a + ih$, $i = 0, \ldots, 2m$, where $h = (b-a)/(2m)$, and let us apply Simpson's rule on each of the intervals $[x_{2i-2}, x_{2i}]$, $i = 1, \ldots, m$, giving

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{i=1}^{m} \int_{x_{2i-2}}^{x_{2i}} f(x)\,dx \\ &\approx \sum_{i=1}^{m} \frac{2h}{6}\left[f\left(x_{2i-2}\right) + 4f\left(x_{2i-1}\right) + f\left(x_{2i}\right)\right]\end{aligned}$$

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Equivalently,

$$\begin{aligned}\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f\left(x_0\right) + 4f\left(x_1\right) + 2f\left(x_2\right) + 4f\left(x_3\right) + \ldots\right. \\ \left. + 2f\left(x_{2m-2}\right) + 4f\left(x_{2m-1}\right) + f\left(x_{2m}\right)\right]\end{aligned}$$

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The numerical integration formula (**??**) is called the composite Simpson rule.

In order to estimate the error in the composite Simpson rule, we proceed in the same way as for the composite trapezium rule:

$$\begin{aligned}
\mathcal{E}_2(f) &:= \int_a^b f(x)\,dx - \sum_{i=1}^{m} \frac{h}{3}\left[f\left(x_{2i-2}\right) + 4f\left(x_{2i-1}\right) + f\left(x_{2i}\right)\right] \\
&= \sum_{i=1}^{m}\left[\int_{x_{2i-2}}^{x_{2i}} f(x)\,dx - \frac{h}{3}\left[f\left(x_{2i-2}\right) + 4f\left(x_{2i-1}\right) + f\left(x_{2i}\right)\right]\right]
\end{aligned}$$

Applying (11) to each individual term under the summation sign and recalling that $b-a=2mh$, we obtain the following error bound:

$$|\mathcal{E}_2(f)| \leq \frac{1}{2880m^4}(b-a)^5 M_4. \tag{15}$$

The composite rules (12) and (**??**) provide greater accuracy than the basic formulae considered in previous section; this is clearly seen by comparing the error bounds (14) and (15) for the two composite rules with (**??**) and (11), the error estimates for the basic trapezium and Simpson formula, respectively.

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