Numerical Methods II

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Numerical Integration

The fundamental problem of numerical integration is the following:
Given the function f continuous on $[a, b]$, approximate

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

Recall that exact integration can be performed using the Fundamental Theorem of Calculus:
If F is an antiderivative of f, that is $F'(x) = f(x)$, then

$$I(f) = \int_a^b f(x)\,dx = F(b) - F(a)$$

Most numerical integration formulas, also known as **quadrature formulas**, are of the form

$$I(f) \approx I_n(f) = \sum_{i=0}^{n} w_i f(x_i)$$

where x_i are the **quadrature points** or **abscissas**, and the w_i are called the **quadrature weights**.

There are two types of quadrature formulas:

Newton-Cotes Quadrature: the quadrature points x_i are fixed and then the weights are obtained by fitting a function to the $f(x_i)$ data;

Gaussian Quadrature: given the number of data points, the weights and quadrature points are selected for maximum accuracy.

Newton-Cotes Quadrature Formulas

The basic procedure is the following:

1. Fix the abscissas $x_0, x_1, x_2 \dots x_n$ in $[a, b]$;
2. Interpolate the function f at these points by the polynomial $P_n(x)$;
3. Integrate the interpolating polynomial to get

$$I(f) \approx I_n(f) \equiv I(P_n)$$

We use the Lagrange interpolating polynomial

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

so the Newton-Cotes quadrature formula is

$$I_n(f) = \sum_{i=0}^{n} w_i f(x_i) \qquad \text{where} \qquad w_i = \int_a^b L_{n,i}(x)\, dx.$$

Lagrange interpolating polynomials

Let $x_0, x_1, x_2, \ldots x_n$ be $n+1$ points and $f_i = f(x_i)$ the function values at these points. An interpolating polynomial P_n is a polynomial of degree at most n such that $P_n(x_i) = f_i$.

The Lagrange Form of the Interpolating polynomial is

$$P_n(x) = \sum_{i=0}^{n} L_{n,i}(x) f_i \qquad \text{where} \qquad L_{n,i}(x) = \prod_{\substack{k=0 \\ k\neq i}}^{n} \frac{x - x_k}{x_i - x_k}$$

Examples (for $n = 1$ and $n = 2$):

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1$$

$$P_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f_2$$

Closed Newton-Cotes formulas

In this case, the abscissas x_i include the endpoints of the interval, a and b. We let Δx denote the length of the (equal) intervals between abscissas and then

$$\Delta x = \frac{b-a}{n} \qquad \text{and} \qquad x_i = a + i\Delta x$$

If $n = 1$ then $x_0 = a$ and $x_1 = b$ and the Lagrange polynomials are

$$L_{1,0}(x) = \frac{b-x}{b-a}, \qquad L_{1,1}(x) = \frac{x-a}{b-a}$$

The closed Newton-Cotes formula for $n = 1$ is

$$I(f) \approx I_1(f) = \frac{\Delta x}{2}\,[f(a) + f(b)] = \frac{b-a}{2}\,[f(a) + f(b)]$$

This is known as the **trapezoidal rule**.

If $n = 2$ then $x_0 = a$, $x_1 = a + \Delta x = \frac{a+b}{2}$ and $x_2 = b$. The quadrature formula for $n = 2$

$$I(f) \approx I_2(f) = \frac{b-a}{6}\left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right]$$

is known as **Simpson's Rule**.

Exercise: Prove the quadrature formulas for $n = 3$ and $n = 4$

$$I_3(f) = \frac{b-a}{8}\left[f(a) + 3f(a+\Delta x) + 3f(a+2\Delta x) + f(b)\right]$$

(The "three-eights rule")

$$I_4(f) = \frac{b-a}{90}\left[7f(a) + 32f(a+\Delta x) + 12f(a+2\Delta x) + 32f(a+3\Delta x) + 7f(b)\right]$$

(Boole's rule)

Open Newton-Cotes Formulas

Open formulas **do not** include the endpoints of the integration interval among abscissas. We have

$$\Delta x = \frac{b-a}{n+2} \qquad \text{and} \qquad x_i = a + (i+1)\Delta x,\ i = 1, n$$

If $n = 0$, $\Delta x = (b-a)/2$ and $x_0 = (a+b)/2$. The open Newton-Cotes quadrature formula is

$$I(f) \approx I_0(f) = (b-a) f\left(\frac{a+b}{2}\right) \qquad \textbf{(The midpoint rule)}$$

If $n = 1$, $\Delta x = (b-a)/3$ and the points are $x_0 = a + \Delta x$ and $x_1 = a + 2\Delta x$. The open Newton-Cotes quadrature formula is

$$I(f) \approx I_1(f) = \frac{(b-a)}{2}\left[f(a+\Delta x) + f(a+2\Delta x)\right].$$

Exercise: Derive the open Newton-Cotes formulas for $n = 2$ and $n = 3$.

Exercise: Approximate the value of the integral

$$I = \int_1^2 \frac{1}{x}\, dx$$

using some of the previous quadrature formulas. Compare the results with the exact value of the integral, $I = \ln(2) = 0.6931...$

Accuracy of quadrature formulas

The degree of precision (or accuracy) of a quadrature rule $I_n(f)$ is the positive integer m such that

- $I(p) = I_n(p)$ for every polynomial p of degree $\leq m$
- $I(p) \neq I_n(p)$ for some polynomial p of degree $m+1$

In other words, the degree of precision is given by the largest integer m such that all polynomials of degree less than m are exactly integrated by the rule.

Note: In practice, we only need to check whether a rule integrates the powers of x exactly. So, if a rule integrates 1, x and x^2 exactly but fails to integrate x^3 exactly, the degree of precision is 2.

Examples

1. The trapezoidal rule integrates 1 and x exactly but fails to integrate x^2 exactly, hence the degree of precision is 1.
2. Verify that Simpson's rule has degree of precision equal to 3.

The following result (given without proof) gives a formula for the error term associated with each Newton-Cotes quadrature rule. This allows for the degree of precision to be calculated.

Error terms

Let $I_n(f)$ denote a Newton-Cotes quadrature rule (open or closed) with $n+1$ abscissas.

- If n is even then there exists a constant c_e and a number ξ_e between a and b such that

$$I(f) = I_n(f) - c_e(b-a)^{n+3} f^{(n+2)}(\xi_e)$$

  Hence the degree of precision of $I_n(f)$ is $n+1$.

- If n is odd, then there exists a constant c_o and a number ξ_o between a and b such that

$$I(f) = I_n(f) - c_o(b-a)^{n+2} f^{(n+1)}(\xi_o)$$

  Hence the degree of precision of $I_n(f)$ is n.

Composite Newton-Cotes quadrature

A composite Newton-Cotes quadrature rule consists of subdividing the integration interval $[a, b]$ into subintervals and then applying low-order Newton-Cotes quadrature formulas on each of the subintervals.

Example: The trapezoidal rule can be written as

$$I(f) = I_1(f) + \text{error} = \frac{b-a}{2}\left[f(a) + f(b)\right] - c(b-a)^3 f''(\xi)$$

We split the integration interval $[a, b]$ into n subintervals

$$a = x_0 \leq x_1 \leq x_2 \leq \cdots x_{n-1} \leq x_n = b$$

where $x_i = a + ih$ for all $0 \leq i \leq n$, and $h = (b-a)/n$.

Apply trapezoidal rule on each interval $[x_{i-1}, x_i]$:

$$I(f) = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)\, dx$$
$$= \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right] - c(b-a)h^2 f''(\xi)$$

where ξ is a number between a and b.

This is the formula for the **composite trapezoidal rule**.

Rates of convergence

Note that $T_h(f)$, the composite trapezoidal rule approximation to the integral $I(f)$ with subintervals of length h, forms a sequence which converges to $I(f)$ as $h \to 0$.

Recall that, if a sequence x_n converges to a limit L such that

$$|x_n - L| \leq C|y_n|, \text{ for all sufficiently large } n$$

where C is a constant and y_n is a sequence which converges to 0 then we say that x_n converges to L with rate of convergence $O(y_n)$.

Easy to see that the rate of convergence for the composite trapezoidal rule is $O(h^2)$.

Exercises

1. Derive the composite Simpson's Rule:

$$I(f) = \frac{h}{3}\left[f(a) + 4\sum_{i=1}^{m} f(x_{2i-1} + 2\sum_{i=1}^{m-1} f(2x_i) + f(b)\right] - c(b-a)h^4 f^{(4)}(\xi),$$

where $n = 2m$. Show that its rate of convergence is $O(h^4)$.

2. Consider the integral

$$I(f) = \int_0^{\pi} \sin(x)\, dx$$

Compute a sequence of approximations $T_h(f)$ (composite trapezoidal rule) and $S_h(f)$ (composite Simpson's rule) which shows clearly the convergence to $I(f)$ and the rates of convergence in each case.

Composite Simpson's Rule

Divide the interval of integration $[a, b]$ into an even number of subintervals, $n = 2m$. Then

$$h = \frac{b-a}{n} = \frac{b-a}{2m} \qquad \text{and} \qquad x_i = a + ih,\ (0 \le i \le 2m)$$

Apply Simpson's rule m times on each interval of the form $[x_{2j-2}, x_{2j}]$ for j between 1 and m.

$$\begin{aligned} I(f) &= \sum_{j=1}^{m} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx \\ &= \frac{h}{3}\left[f(x_0) + 4\sum_{j=1}^{m} f(x_{2j-1}) + 2\sum_{j=1}^{m-1} f(x_{2j}) + f(x_{2m})\right] - c(b-a)h^4 f^{(4)}(\xi) \end{aligned}$$

Numerical verification of rate of convergence

We verified numerically, using the integral

$$I(f) = \int_0^{\pi} \sin(x)\, dx = 2,$$

that the composite trapezoidal rule has rate of convergence $O(h^2)$ and and the composite Simpson's rule has rate of convergence $O(h^4)$.

This was achieved by showing that $\dfrac{e_{2h}}{e_h} \to 4$ as $h \to 0$, for the trapezoidal rule and $\dfrac{e_{2h}}{e_h} \to 16$ as $h \to 0$ for Simpson's rule.

If the exact value of the integral $I(f)$ is not known then the rates of convergence can be verified by showing that

$$\frac{T_h(f) - T_{h/2}(f)}{T_{h/2}(f) - T_{h/4}(f)} \to 4 \qquad \text{as } h \to 0$$

for the composite trapezoidal rule, and

$$\frac{S_h(f) - S_{h/2}(f)}{S_{h/2}(f) - S_{h/4}(f)} \to 16 \qquad \text{as } h \to 0$$

for the composite Simpson's rule.

Example:

Using the integral

$$I(f) = \int_0^1 \sqrt{1+x^3}\,dx$$

verify numerically that the composite trapezoidal rule has rate of convergence $O(h^2)$.

Application: Using error terms

It can be shown that the error term for the composite trapezoidal rule can be more accurately expressed as

$$e_h = \frac{(b-a)h^2}{12} f''(\xi) = \frac{(b-a)^3}{12n^2} f''(\xi), \qquad a \leq \xi \leq b,$$

while the error term for the composite Simpson's rule is

$$e_h = \frac{(b-a)h^4}{180} f''(\xi) = \frac{(b-a)^5}{180n^4} f''(\xi), \qquad a \leq \xi \leq b,$$

Example

Using the integral

$$\int_0^1 \frac{1}{1+x^2}\,dx = \frac{\pi}{4}$$

determine the number of subintervals needed for the composite trapezoidal rule and the composite Simpson's rule in order to approximate π to four decimal places.

We must have

$$e_h = |I(f) - T_h(f)| < 1.25 \times 10^{-5}$$

and we can show that, if $f(x) = \frac{1}{1+x^2}$ then

$$\max_{x\in[0,1]} |f''(x)| = 2 \qquad \text{and} \qquad \max_{x\in[0,1]} |f^{(4)}(x)| = 24$$

For the trapezoidal rule we must select n so that

$$e_h = \frac{(1-0)^3}{12n^2} \cdot 2 < 1.25 \times 10^{-5}$$

so $n \geq 116$.

For Simpson's rule we must select n so that

$$e_h = \frac{(1-0)^5}{180n^4} \cdot 24 < 1.25 \times 10^{-5}$$

so $n \geq 12$.

Gaussian quadrature

Recall that Newton-Cotes formulae are based on equally spaced quadrature points of the form $x_i = a + ih$, where $h = (b-a)/n$. By contrast, Gaussian quadrature rules make an adaptive choice of nodes that minimizes the approximation error and therefore has maximum possible degree of precision for any rule using n points.

To develop such rule, we use the **method of undetermined coefficents**: We need to find the numbers $x_1, x_2, \ldots x_n$ (the abscissas) and $w_1, w_2, \ldots w_n$ (the weights) such that the approximation

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

has degree of precision $2n-1$, in other words it integrates the polynomials 1, x, x^2, ..., x^{2n-1} exactly.

One-point Gaussian quadrature rule

The approximation formula

$$\int_a^b f(x)\,dx = w_1 f(x_1)$$

has degree of precision equal to 1 if it integrates 1 and x exactly, that is

$$b - a = w_1 \quad \text{and} \quad \frac{1}{2}(b^2 - a^2) = w_1 x_1$$

We get $w_1 = b - a$ and $x_1 = (a + b)/2$ so the quadrature rule is the midpoint rule:

$$\int_a^b f(x)\,dx = (b - a)\, f\left(\frac{a + b}{2}\right)$$

Two-point Gaussian quadrature rule

First convert the integral $\int_a^b f(x)\,dx$ into an integral over $[-1,1]$.

The change of variables

$$x = \frac{b-a}{2}\,t + \frac{a+b}{2}$$

gives

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}t + \frac{a+b}{2}\right)dt$$

The two-point quadrature rule

$$\int_{-1}^{1} f(t)\,dt \approx w_1 f(t_1) + w_2 f(t_2)$$

has degree of precision $2\cdot 2-1=3$ if the following equations hold:

$$\begin{aligned} w_1 + w_2 &= 2 \\ w_1 t_1 + w_2 t_2 &= 0 \\ w_1 t_1^2 + w_2 t_2^2 &= \frac{2}{3} \\ w_1 t_1^3 + w_2 t_2^3 &= 0 \end{aligned}$$

The two-point quadrature rule becomes

$$\int_{-1}^{1} f(t)\,dt \approx f\left(-\sqrt{\frac{1}{3}}\right) + f\left(\sqrt{\frac{1}{3}}\right)$$

The error term can be shown to be equal to

$$\frac{1}{135} f^{(4)}(\xi), \quad \text{where} \quad -1 < \xi < 1.$$

Converting back to the original interval we get

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\left[f\left(\frac{a+b}{2} - \sqrt{\frac{1}{3}}\frac{b-a}{2}\right) + f\left(\frac{a+b}{2} + \sqrt{\frac{1}{3}}\frac{b-a}{2}\right)\right]$$
$$+\frac{(b-a)^5}{4320} f^{(4)}(\hat{\xi}), \qquad \text{where} \quad a < \hat{\xi} < b$$

Example: Consider the integral

$$I = \int_{-1}^{1} e^{x} \sin(\pi x)\, dx = \frac{\pi(e^2 - 1)}{e(\pi^2 + 1)} \approx 0.679326$$

Compare the errors obtained when approximating this integral with Simpson's rule and the two-point Gaussian rule above.

Example: Using the two-point Gaussian quadrature formula, approximate the integrals

$$\text{(i)} \int_{-1}^{1} e^{-x}\, dx; \qquad \text{(ii)} \int_{0}^{\pi} \sin(x)\, dx$$

and find the absolute error in each case.

Composite two-point Gaussian rule

Let $h = (b-a)/n$ and $x_i = a = ih$ for $i = 1, \ldots n$. Applying the basic Gaussian rule on each interval $[x_{i-1}, x_i]$ show that the composite Gaussian quadrature rule is

$$\int_a^b f(x)\,dx = \frac{h}{2}\sum_{i=1}^{n}\left[f\left(x_i - \frac{h}{2} - \sqrt{\frac{1}{3}}\frac{h}{2}\right) + f\left(x_i - \frac{h}{2} + \sqrt{\frac{1}{3}}\frac{h}{2}\right)\right] + \frac{(b-a)h^4}{4320}\,f^{(4)}(\xi)$$

Three-point Gaussian rule

Derive the three-point Gaussian rule:

$$\int_{-1}^{1} f(x)\,dx \approx \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$$

and convert this formula to the general integration interval $[a, b]$.

Example: Using the three-point Gaussian quadrature formula, approximate the integrals

$$\text{(i)} \int_{-1}^{1} \mathrm{e}^{-x}\,dx; \qquad \text{(ii)} \int_{0}^{\pi} \sin(x)\,dx$$

and find the absolute error in each case.