Computational method and numerical algorithms: Lecture 6

Wangtao Lu
Zhejiang University

October 20, 2020

Contents

Wangtao Lu
Zhejiang University

Chapter 5: numerical differentiation and integration

the purpose of this chapter is to develop numerical methods to numerically compute

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

when $f(x)$ is given on $[a, b]$.

5.1 Numerical Differentiaiton

We first discuss finite difference formulas for approximating derivatives.

Finite Difference Formulas

1. Two-point forward-difference formula

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi), \quad \xi \in (x, x+h).$$

2. Three-point centered-difference formula

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(\xi), \quad \xi \in (x-h, x+h).$$

3. Three-point centered-difference formula for second derivative

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi), \quad \xi \in (x-h, x+h).$$

Example 1. Use the above formulas to find $f'(2)$ and $f''(2)$ for $f(x) = 1/x$ with $h = 0.1$.

Rounding error

Example 2. Approximate the derivative of $f(x) = e^x$ at $x = 0$.
Sol. The two-point formula gives

$$f'(0) \approx \frac{e^{0+h} - e^0}{h}, \tag{1}$$

while the three-point formula gives

$$f'(0) \approx \frac{e^h - e^{-h}}{h}. \tag{2}$$

Trying different values of h, we get the following table,

h	Error in (1)	Error in (2)
10^{-1}	$-5.17e-2$	$-1.67e-3$
10^{-2}	$-5.01e-3$	$-1.67e-5$
10^{-3}	$-5.00e-4$	$-1.67e-7$
10^{-4}	$-5.00e-5$	$-1.67e-9$
10^{-5}	$-5.00e-6$	$-1.21e-11$
10^{-6}	$-5.00e-7$	$-2.67e-11$
10^{-7}	$-4.94e-8$	$-5.26e-10$
10^{-8}	$-6.08e-9$	$-6.08e-9$
10^{-9}	$-8.27e-8$	$-2.72e-8$

Error Analysis for two-point formula

Two-point formula:

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{f''(\xi)h}{2}, \quad \xi \in (x, x+h),$$

Machine Approximation:

$$f'(x)_{\mathrm{MACH}} = \frac{\hat{f}(x+h) - \hat{f}(x)}{h},$$

where $\hat{f}(x)$ is the machine output of $f(x)$, such that

$$|\hat{f}(x) - f| \leq \epsilon_1, \quad |\hat{f}(x+h) - f(x+h)| \leq \epsilon_2.$$

Thus,

$$\mathrm{Err}(h) = |f'(x) - f'(x)_{\mathrm{MACH}}| \leq \frac{\epsilon_1 + \epsilon_2}{h} + \frac{f''(\xi)h}{2} \leq \frac{\epsilon_1 + \epsilon_2}{h} + \frac{Mh}{2}.$$

When the error bound attains its minimum? Differentiate it w.r.t h:

$$\frac{M}{2} - \frac{\epsilon_1 + \epsilon_2}{h^2} = 0 \rightarrow h = \sqrt{\frac{2(\epsilon_1 + \epsilon_2)}{M}}.$$

If $\epsilon_1 = \epsilon_2 = \epsilon_{\mathrm{MACH}} = 2.2 \times 10^{-16}$, we approximately get $h \approx \mathcal{O}(10^{-8})$.

Extrapolation

Assume that we have an order n formula $F(h)$ for approximating a given quantity Q, i.e.,

$$Q \approx F(h) + Kh^n.$$

Richardson extrapolation indicates that

$$Q \approx \frac{2^n F(h/2) - F(h)}{2^n - 1} + \mathcal{O}(h^{n+1}).$$

Example 1. Apply this to the three-point formula for first-order derivative.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(\xi), \quad \xi \in (x-h, x+h).$$

Then,

$$F(h) = \frac{f(x+h) - f(x-h)}{2h}, \quad n = 2,$$

such that

$$\frac{2^n F(h/2) - F(h)}{2^n - 1} = \frac{f(x-h) - 8f(x-h/2) + 8f(x+h/2) - f(x+h)}{6h},$$

is of order at least three. In fact, it has order four by Taylor's Residual Theorem.

5.2 Numerical Integration

Given a function f on $[a, b]$, find $\int_a^b f(x)dx$. We will introduce three types of rules:

- Trapezoid Rule
- Simpson's Rule
- Midpoint Rule

Based on the composition of the above rules, we will develop Newton-Cotes Formulas.

Wangtao Lu
Zhejiang University

Trapezoid Rule

For a given function f on an interval $[x_0, x_1]$ of a small length $h = x_1 - x_0$, we can use the linear interpolating polynomial to approximate f with an error function $E(x)$, i.e.,

$$f(x) = f(x_0)\frac{x - x_1}{x_0 - x_1} + f(x_1)\frac{x - x_0}{x_1 - x_0} + \frac{(x - x_0)(x - x_1)}{2!} f''(\xi(x)) = P(x) + E(x)$$

Then, we have

$$\int_{x_0}^{x_1} f(x)dx = \int_{x_0}^{x_1} P(x)dx + \int_{x_0}^{x_1} E(x)dx.$$

One easily derives that

$$\int_{x_0}^{x_1} P(x)dx = \frac{h}{2}(f(x_0) + f(x_1)), \quad \int_{x_0}^{x_1} E(x)dx = -\frac{h^3}{12} f''(c),$$

for some $c \in [x_0, x_1]$. Thus, we have obtained Trapezoid Rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{h^3}{12} f''(c).$$

Simpson's Rule

For a given function f on a small interval $[x_0, x_2]$ of length $x_2 - x_0 = 2h$, we can use the interpolating porabola to approximate f by

$$\begin{aligned} f(x) =& \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \\ &+ \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{3!} f'''(\xi) \\ =& P(x) + E(x). \end{aligned}$$

Using this, we can approximate

$$\int_{x_0}^{x_2} f(x)dx = \int_{x_0}^{x_2} P(x)dx + \int_{x_0}^{x_2} E(x)dx,$$

so that one easily derives the **Simpson's Rule**:

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

for some $c \in [x_0, x_2]$.

Midpoint Rule

One similarly gets the following **Midpoint Rule** from Trapezoid Rule:

$$\int_{x_0}^{x_1} f(x)dx = hf\left(\frac{x_0 + x_1}{2}\right) + \frac{h^3}{24} f''(c).$$

An advantage of Midpoint Rule over Trapezoid Rule is when $f(x)$ is singular at x_0 or x_1, the Midpoint Rule still applies whereas Trapezoid Rule doesn't.

Example 1. Apply the Trapezoid Rule, Simpson's Rule, and Midpoint Rule to approximate

$$\int_1^2 \ln x dx,$$

and find an upper bound for the error in your approximation.

Degree of Precision of A Numerical Integration Method

The degree of precision of a numerical integration method is the greatest integral k for which all degree k or less polynomials are integrated exactly by the method.
For example,

- The degree of precision of trapezoid Rule is .

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{h^3}{12}f''(c).$$

- The degree of precision of Simpson's Rule is

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

- The degree of precision of Midpoint Rule is

$$\int_{x_0}^{x_1} f(x)dx = hf\left(\frac{x_0 + x_1}{2}\right) + \frac{h^3}{24}f''(c).$$

Degree of Precision of A Numerical Integration Method

The degree of precision of a numerical integration method is the greatest integral k for which all degree k or less polynomials are integrated exactly by the method.
For example,

- The degree of precision of trapezoid Rule is 1.

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f(x_0)+f(x_1)) - \frac{h^3}{12}f''(c).$$

- The degree of precision of Simpson's Rule is

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

- The degree of precision of Midpoint Rule is

$$\int_{x_0}^{x_1} f(x)dx = hf\left(\frac{x_0+x_1}{2}\right) + \frac{h^3}{24}f''(c).$$

Degree of Precision of A Numerical Integration Method

The degree of precision of a numerical integration method is the greatest integral k for which all degree k or less polynomials are integrated exactly by the method.
For example,

- The degree of precision of trapezoid Rule is 1.

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{h^3}{12}f''(c).$$

- The degree of precision of Simpson's Rule is 3

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

- The degree of precision of Midpoint Rule is

$$\int_{x_0}^{x_1} f(x)dx = hf\left(\frac{x_0 + x_1}{2}\right) + \frac{h^3}{24}f''(c).$$

Degree of Precision of A Numerical Integration Method

The degree of precision of a numerical integration method is the greatest integral k for which all degree k or less polynomials are integrated exactly by the method.
For example,

- The degree of precision of trapezoid Rule is 1.

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{h^3}{12} f''(c).$$

- The degree of precision of Simpson's Rule is 3

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

- The degree of precision of Midpoint Rule is 1

$$\int_{x_0}^{x_1} f(x)dx = hf\left(\frac{x_0 + x_1}{2}\right) + \frac{h^3}{24} f''(c).$$

Example 2. Find the degree of precision of the degree 3 Newton-Cotes formula, called the **Simpson's** $3/8$ **Rule**:

$$\int_{x_0}^{x_3} f(x)dx \approx \frac{3h}{8}(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)).$$

Composite Newton-Cotes formulas

1. Divide the interval of integration into a number of subintervals;
2. On each subinterval, we apply one of the Trapezoid, Simpson's, or Midpoint Rule to approximate the integral over this subinterval.

Composite Trapezoid Rule

To approximate

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

we first divide $[a, b]$ into a number of subintervals. Consider the following evenly spaced grid

$$a = x_0 < x_1 < x_2 < \cdots < x_{m-2} < x_{m-1} < x_m = b,$$

where $h = x_{i+1} - x_i$ for all $i = 0, \ldots, m-1$. On each panel/subinterval $[x_i, x_{i+1}]$, we use Trapezoid Rule to approximate

$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}(f(x_i) + f(x_{i+1})) - \frac{h^3}{12} f''(\xi_i),$$

then we get

$$\int_a^b f(x) = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{m-1} f(x_i)\right] - \sum_{i=0}^{m-1} \frac{h^3}{12} f''(\xi_i).$$

Consequently, we get the **Composite Trapezoid Rule**

$$\int_a^b f(x) = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{m-1} f(x_i)\right] - \frac{(b-a)h^2}{12} f''(c),$$

for some $c \in [a, b]$.

Composite Simpson's Rule

To approximate

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

we first divide $[a, b]$ into a number of subintervals. Consider the following evenly spaced grid

$$a = x_0 < x_1 < x_2 < \cdots < x_{2m-2} < x_{2m-1} < x_{2m} = b,$$

where $h = x_{i+1} - x_i$ for all $i = 0, \ldots, 2m-1$. On each length $2h$ panel $[x_{2i}, x_{2i+2}]$, we use Simpson's Rule to approximate

$$\int_{x_{2i}}^{x_{2i+2}} f(x)dx = \frac{h}{3}(f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})) - \frac{h^5}{90} f''(\xi_i),$$

then we get

$$\int_a^b f(x) = \frac{h}{3}\left[f(a) + f(b) + 4\sum_{i=1}^{m} f(x_{2i-1}) + 2\sum_{i=1}^{m-1} f(x_{2i})\right] - \sum_{i=0}^{m-1} \frac{h^5}{90} f^{(4)}(\xi_i),$$

so that we obtain the Composite Simpson's Rule

$$\int_a^b f(x) = \frac{h}{3}\left[f(a) + f(b) + 4\sum_{i=1}^{m} f(x_{2i-1}) + 2\sum_{i=1}^{m-1} f(x_{2i})\right] - \frac{(b-a)h^4}{180} f^{(4)}(c),$$

for some $c \in [a, b]$.

Example 2. Carry out four-panel approximations of

$$\int_1^2 \ln x dx$$

using the composite Trapezoid Rule and composite Simpson's Rule.

Example 3. Find the number of panels m necessary for the composite Simpson's Rule to approximate

$$\int_0^{\pi} \sin^2 x dx$$

within six correct decimal places.

Composite Midpoint Rule

To approximate

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

we first divide $[a, b]$ into a number of subintervals. Consider the following evenly spaced grid

$$a = x_0 < x_1 < x_2 < \cdots < x_{m-2} < x_{m-1} < x_m = b,$$

where $h = x_{i+1} - x_i$ for all $i = 0, \ldots, m-1$. On each panel/subinterval $[x_i, x_{i+1}]$, we use Midpoint Rule to approximate

$$\int_{x_i}^{x_{i+1}} f(x)dx = hf(w_{i+1}) + \frac{h^3}{24} f''(\xi_{i+1}),$$

where $w_i = \frac{x_{i+1}+x_i}{2}$, then we get

$$\int_a^b f(x) = h\sum_{i=1}^{m} f(w_i) + \sum_{i=1}^{m} \frac{h^3}{24} f''(\xi_{i+1}).$$

Consequently, we get the **Composite Midpoint Rule**

$$\int_a^b f(x) = h\sum_{i=1}^{m} f(w_i) + \frac{(b-a)h^2}{24} f''(c),$$

for some $c \in [a, b]$.

Example 3. Approximate

$$\int_0^1 \frac{\sin x}{x} dx$$

by using the Composite Midpoint Rule with $m = 10$ panels.

Orthogonal Polynomials

The set of nonzero functions $\{p_0, \ldots, p_n\}$ on the interval $[a, b]$ is **orthogonal** on $[a, b]$ if

$$\int_a^b p_j(x)p_k(x) = \begin{cases} 0 & j \neq k, \\ \neq 0 & j = k. \end{cases}$$

Theorem. If $\{p_0, p_1, \ldots, p_n\}$ is an orthogonal set of polynomials on the interval $[a, b]$, where $\deg p_i = i$, then $\{p_0, p_1, \ldots, p_n\}$ is a basis for the vector space of degree at most n polynomials on $[a, b]$.

Theorem. If $\{p_0, \ldots, p_n\}$ is an orthogonal set of polynomials on $[a, b]$ and if $\deg p_i = i$, then p_i has i distinct roots in the interval (a, b).

Example 1. Find a set of three orthogonal polynomials on the interval $[-1,1]$.

Legendre Polynomials

Example 2. Show that the set of **Legendre Polynomials**

$$P_i(x) = \frac{1}{2^i}\frac{d^i}{dx^i}[(x^2-1)^i]$$

for $0 \leq i \leq n$ is orthogonal on $[-1, 1]$.

Properties of Legendre Polynomials

Prop. 1. Recursive relation:

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x), n \geq 1.$$

The first few are

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= \frac{1}{2}(3x^2 - 1). \end{aligned}$$

Prop. 2 $P_n(1) = 1$, $n \geq 0$.
Prop. 3 $P_n(x)$ is of degree n and has n distinct roots in $[-1, 1]$.

Gaussian Quadrature

For a given function f on $[-1,1]$. Suppose the n distinct roots of degree n Legendre Polynomial $P_n(x)$ are

$$x_1, x_2, \ldots, x_n \in [-1,1],$$

then, we could find a polynomial of degree $n-1$ or less to interpolate f at $x_1, \ldots, x_n$,

$$f(x) \approx \sum_{i=1}^{n} f(x_i) L_i(x),$$

where

$$L_i(x) = \frac{\prod_{j\neq i}(x - x_j)}{\prod_{j\neq i}(x_i - x_j)}.$$

Then, we have the following **Gaussian-Legendre Quadrature**

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i),$$

where

$$c_i = \int_{-1}^{1} L_i(x).$$

What is the degree of precision of Gaussian Quadrature? The interpolating error formula indicates that the answer is $n-1$.

Main Theorem

Theorem. The Gaussian Quadrature Method, using the degree n Legendre polynomial on $[-1,1]$, has **degree of precision** $2n-1$.

Proof. Let $P(x)$ be a polynomial of degree at most $2n-1$. We must show that

$$\int_{-1}^{1} P(x)dx = \sum_{i=1}^{n} c_i P(x_i).$$

Using long division of polynomials, we can express

$$P(x) = S(x)P_n(x) + R(x),$$

where $S(x)$ and $R(x)$ are polynomials of degree less than n. Thus, we easily see that

$$\int_{-1}^{1} R(x)dx =$$

And since

$$\int_{-1}^{1} S(x)P_n(x)dx = 0,$$

which completes the proof.

Main Theorem

Theorem. The Gaussian Quadrature Method, using the degree n Legendre polynomial on $[-1, 1]$, has **degree of precision** $2n - 1$.

Proof. Let $P(x)$ be a polynomial of degree at most $2n - 1$. We must show that

$$\int_{-1}^{1} P(x)dx = \sum_{i=1}^{n} c_i P(x_i).$$

Using long division of polynomials, we can express

$$P(x) = S(x)P_n(x) + R(x),$$

where $S(x)$ and $R(x)$ are polynomials of degree less than n. Thus, we easily see that

$$\int_{-1}^{1} R(x)dx = \sum_{i=1}^{n} c_i R(x_i) = \sum_{i=1}^{n} c_i P(x_i).$$

And since

$$\int_{-1}^{1} S(x)P_n(x)dx = 0,$$

which completes the proof.

Main Theorem

Theorem. The Gaussian Quadrature Method, using the degree n Legendre polynomial on $[-1, 1]$, has **degree of precision** $2n-1$.

Proof. Let $P(x)$ be a polynomial of degree at most $2n-1$. We must show that

$$\int_{-1}^{1} P(x)dx = \sum_{i=1}^{n} c_i P(x_i).$$

Using long division of polynomials, we can express

$$P(x) = S(x)P_n(x) + R(x),$$

where $S(x)$ and $R(x)$ are polynomials of degree less than n. Thus, we easily see that

$$\int_{-1}^{1} R(x)dx = \sum_{i=1}^{n} c_i R(x_i) = \sum_{i=1}^{n} c_i P(x_i).$$

And since $S(x)$ and $P_n(x)$ are orthogonal to each other, we have

$$\int_{-1}^{1} S(x)P_n(x)dx = 0,$$

which completes the proof.

Example 3. Approximate

$$\int_{-1}^{1} e^{-x^2/2} dx,$$

using Gaussian Quadrature.

Change of interval

What if we are integrating f on $[a, b]$? We can directly use the method of change of variables!

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

Contents

Wangtao Lu
Zhejiang University

Assignment VI

Assignment VI:
5.1 P254, Computer Problems: 1.
5.2 P264, Computer Problems: 1.(a,c) (Note: Using Composite Trapezoid and Simpson report the errors by using $m = 16$ and 32 panels.), 7(c).
5.5 P278, Exercises: 3. (Note: just do (a) and use Matlab (not your hand) to do the computations!)
Due date: November 3, 2020.

Wangtao Lu
Zhejiang University