MA2252 Introduction to computing

lectures 27-28

Numerical derivation and numerical integration

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Numerical derivation

For a function $f(x)$, the slope of a secant line passing through points $(a, f(a))$ and $(a+h, f(a+h))$ is

$$slope = \frac{f(a+h) - f(a)}{h}.$$

When $h \to 0$, this slope becomes the derivative of a function $f(x)$ at $x = a$:

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}. \tag{1}$$

Introduction (contd.)

Points to note ☛

- (1) is helpful if analytical form of $f(x)$ is known explicitly.
- Even if $f(x)$ is known, sometimes analytical form of f'(x) can be too complicated.

Finite-difference schemes

- The domain of a function $f(x)$ can be represented by a **numerical grid** which contains points x_i evenly spaced by fixed distance called **spacing** or **step size**.
- A **finite difference** is the difference of values of function $f(x)$ at two grid points. MATLAB's diff() operator finds the finite differences $f(x_{i+1}) - f(x_i)$.
- A **finite-difference scheme** for derivative provides a formula for estimating derivative of a function on the numerical grid.

Finite-difference schemes (contd.)

Some finite difference schemes:

- Forward difference

$$f'(a) \approx \frac{f(a+h) - f(a)}{h}. \tag{2}$$

- Backward difference

$$f'(a) \approx \frac{f(a) - f(a-h)}{h}. \tag{3}$$

- Central difference

$$f'(a) \approx \frac{f(a+h) - f(a-h)}{2h}. \tag{4}$$

Taylor series approximations of derivatives

The finite difference schemes discussed before can also be derived using Taylor series. Consider the Taylor series of a function $f(x)$ at $x = a$:

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots \tag{7}$$

which for the point $x = a + h$ gives

$$f(a+h) = f(a) + \frac{f'(a)}{1!}h + \frac{f''(a)}{2!}h^2 + \cdots . \tag{8}$$

From (8), we have

$$f'(a) = \frac{f(a+h) - f(a)}{h} - \frac{f''(a)}{2!}h - \frac{f'''(a)}{3!}h^2 + \cdots . \tag{9}$$

For very small h, (9) gives the approximation

$$f'(a) \approx \frac{f(a+h) - f(a)}{h} \tag{10}$$

Exercise: Derive backward and central difference schemes for $f'(a)$ using Taylor series of $f(x)$.

The Big O notation

Consider equation (10) again.

$$f'(a) = \frac{f(a+h) - f(a)}{h} - \frac{f''(a)}{2!}h - \frac{f'''(a)}{3!}h^2 + \cdots . \qquad (11)$$

This can be compactly written as

$$f'(a) = \frac{f(a+h) - f(a)}{h} + O(h). \qquad (12)$$

Let's now study what $O(h)$ means.

The Big O notation (contd.)

Let $\phi(h) = -\frac{f''(a)}{2!}h - \frac{f'''(a)}{3!}h^2 + \cdots$.

Then

$$\lim_{h \to 0} \frac{\phi(h)}{h} = -\frac{f''(a)}{2!} = C(say) \tag{15}$$

which means

$$\phi(h) = O(h) \quad \text{as} \quad h \to 0 \tag{16}$$

Thus, we say that forward difference scheme (12) is $O(h)$.

Order of accuracy

For a $O(h^p)$ finite difference scheme, p is called the **order of accuracy**.

Example: The forward difference scheme (12) is first order accurate.

Exercise: Show that the central difference scheme for $f'(a)$ can be written as

$$f'(a) = \frac{f(a+h) - f(a-h)}{2h} + O(h^2) \tag{17}$$

and therefore is second order accurate.

Higher order derivatives

We can again use Taylor series to approximate higher order derivatives of $f(x)$.

Example: Find finite-difference scheme for $f''(a)$.

For points $x = a + h$ and $x = a - h$ from (8) we have

$$f(a+h) = f(a) + \frac{f'(a)}{1!}h + \frac{f''(a)}{2!}h^2 + \cdots . \tag{18}$$

$$f(a-h) = f(a) - \frac{f'(a)}{1!}h + \frac{f''(a)}{2!}h^2 + \cdots . \tag{19}$$

Higher order derivatives (contd.)

Adding equations (18) and (19) and solving for $f''(a)$ gives

$$f''(a) \approx \frac{f(a+h) - 2f(a) + f(a-h)}{h^2} \tag{20}$$

Numerical integration

Why study numerical integration?

- The anti-derivatives of many functions cannot be represented in terms of elementary functions. **Examples:** $\frac{\sin x}{x}$, e^{-x^2} and $\frac{1}{\ln x}$
- Analytical form of the integrand function(say $f(x)$) may be unknown. **Example:** The values of $f(x)$ are only known at a set of data points x_i.

Problem statement

Consider a function $f(x)$ defined over a interval $[a, b]$. We want to evaluate

$$I = \int_a^b f(x)dx. \tag{1}$$

This integral can be geometrically seen as area under the curve $y = f(x)$ for $x \in [a, b]$.

Problem statement (contd.)

Steps to evaluate (1) numerically:

- Create a numerical grid $x_i \quad (i = 0, 1, 2, \cdots, n)$ such that $x_0 = a, x_n = b$ and $x_{i+1} - x_i = h$(say).
- Using some appropriate method, calculate the area A_i under $f(x)$ for each sub-interval $[x_i, x_{i+1}] \quad (i = 0, 1, 2, \cdots, n-1)$.
- Compute the sum of the areas A_i over the interval $[a, b]$ i.e.

$$I \approx \sum_{i=0}^{n-1} A_i \tag{2}$$

Numerical integration methods

- Midpoint rule
- Trapezoidal rule
- Simpson's rule

Midpoint rule

Steps:

- The value of function in a subinterval $[x_i, x_{i+1}]$ is interpolated by a constant function with the value $f(\frac{x_i+x_{i+1}}{2})$.
- The area A_i is calculated by area of rectangle under the constant function.

$$A_i = h * f(\frac{x_i + x_{i+1}}{2}) \tag{3}$$

Midpoint rule (contd.)

Example: Write a script file which uses Midpoint rule to approximate $\int_0^{\pi} \sin x \, dx$.

Trapezoidal rule

Steps:

- Here, the function in the subinterval $[x_i, x_{i+1}]$ is approximated using a straight line joining points $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$ (linear interpolation).
- The area A_i is calculated by the area of trapezium formed under this straight line.

$$A_i = \frac{1}{2}(f(x_i) + f(x_{i+1}))h \tag{4}$$

Simpson's rule

Steps:

- Here, the function $f(x)$ is approximated on two subintervals $[x_{i-1}, x_i]$ and $[x_i, x_{i+1}]$ taken together. The interpolating function is a quadratic passing through points $(x_{i-1}, f(x_{i-1}))$, $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$.

- The area B_i over interval $[x_{i-1}, x_{i+1}]$ is derived as

$$B_i = \frac{h}{3}(f(x_{i-1}) + 4f(x_i) + f(x_{i+1})) \tag{5}$$

- The integral I is given by

$$I \approx \sum_{i=1, i=odd}^{n-1} B_i \tag{6}$$

Simpson's rule (contd.)

(6) can also be expressed in the form:

$$I \approx \frac{h}{3}\left[f(x_0) + 4\left(\sum_{i=1, i=odd}^{n-1} f(x_i) \right) + 2\left(\sum_{i=2, i=even}^{n-2} f(x_i) \right) + f(x_n) \right] \quad (7)$$

Note: Since B_i is calculated for two consecutive subintervals taken together, Simpson's rule requires even number of subintervals i.e. n should be even.

MATLAB's built-in integration functions

Two useful functions are trapz() and integral().

- trapz(x,f) takes of numerical grid x and function f as vector arguments and computes the value of integral I using trapezoidal rule.

- integral(fun,xmin,xmax) integrates the function fun from lower limit xmin to upper limit xmax.