MA2252 Introduction to Computing

Lecture 17
Numerical Differentiation

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Learning outcomes

At the end of lecture, students will be able to

- finite difference schemes for derivatives
- understand Taylor series approximations for derivatives
- use MATLAB to find derivatives numerically

Introduction

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 $x = a$:

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

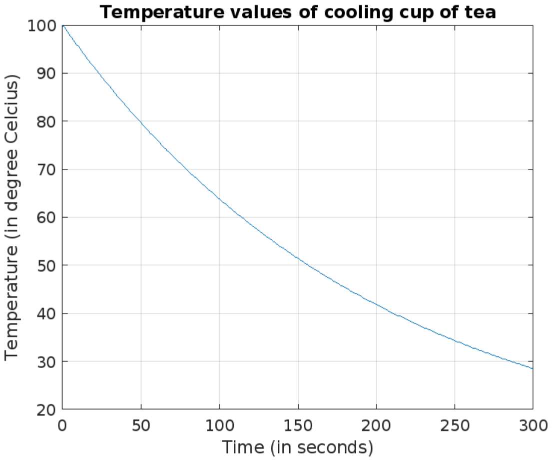
Introduction (contd.)

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.

Introduction (contd.)

Example: Suppose you go outside with a cup of tea heated at 100 °C. The outside temperature is 8 °C. What is the rate of cooling at any time instant?



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

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

Finite-difference schemes (contd.)

Example: Write a script file which uses finite difference schemes to plot the temperature gradient curve for the cooling cup of tea example.

Demo

Finite-difference schemes (contd.)

The analytical form of $T(t)$ comes from Physics. For our problem, it is taken as

$$T = 8 + 92e^{-0.005t} \tag{5}$$

The exact solution for temperature gradient is given by

$$\frac{dT}{dt} = -0.46e^{-0.005t} \tag{6}$$

Example: Write a script file to plot the exact and approximate temperature gradient of cup of tea example.

Finite-difference schemes (contd.)

Demo

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

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

Taylor series approximations of derivatives (contd.)

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.

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

This can be compactly written as

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

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

The Big O notation (contd.)

Definition

For two functions $\phi(x)$ *and* $\psi(x)$,

$$\phi(x) = O(\psi(x)) \quad \textit{as} \quad x \to x_0 \tag{13}$$

if

$$\lim_{x \to x_0} \frac{\phi(x)}{\psi(x)} = C \tag{14}$$

where C *is a finite constant.*

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

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

End of Lecture 17

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