MA2252 Introduction to Computing

Lecture 17
Numerical Differentiation

Sharad Kumar Keshari

School of Computing and Mathematical Sciences

University of Leicester

Learning outcomes

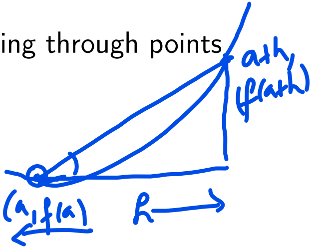
At the end of lecture, students will be able to

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

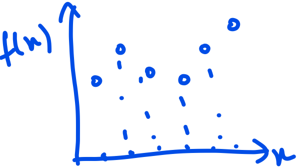
Introduction

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

$$\underbrace{slope}_{\text{of secant}} = \frac{f(a+h) - f(a)}{h}.$$



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.)

$$f(x) = \sqrt{\sin x} \times \log x \times e^{-x^2}$$

$f'(x)$ vs x

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.

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?

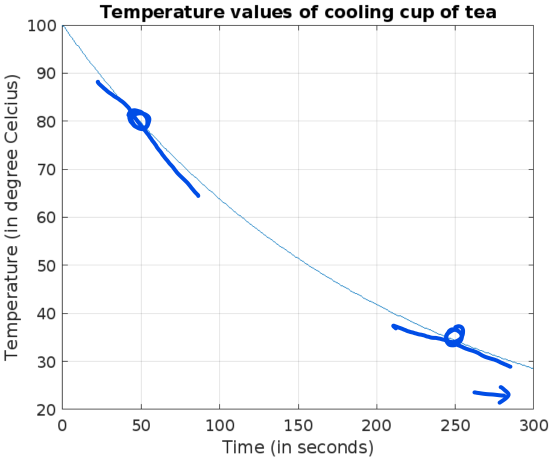
rate of change of temp. with time $= \frac{dT}{dt}$

$\parallel$

temperat[ure]

the

gradient



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 $f(x_{i+1}) - f(x_i)$.

  or method

- 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:

$\frac{1}{2}(a+b)$

- Forward difference

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

- Backward difference

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

- Central difference

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

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

Demo

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

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

Newton's law of cooling

The exact solution for temperature gradient is given by

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

$$T = \underset{\underset{8}{\parallel}}{T_a} + \underbrace{(T_0 - T_a)}_{(100-8)} e^{-\underbrace{r}_{\text{heat transfer coefficient}} t}$$

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 $f(x)$.

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

order

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

Big 'O' notation

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

The Big O notation (contd.)

Definition

For two functions $\phi(x)$ and $\psi(x)$, ϕ is of order of ψ as $x \to x_0$

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

x_0 can be finite, ∞, $-\infty$

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.

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

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

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

$f(a+h) + f(a-h) - 2f(a) = f''(a)h^2 + \cdots$

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

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

$O(h)$?

$O(h^2)$?

$O(h^4)$?

$f(a-h)$ $f(a)$ $f(a+h)$

$f'''(a) = ?$

$f''''(a) = ?$

End of Lecture 17

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