HUST

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HANOI UNIVERSITY OF SCIENCE AND TECHNOLOGY

ONE LOVE. ONE FUTURE.

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Chapter 5: Derivative and Integral

Scientific Computing

SoICT 2023

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Content

1. Approximation of Derivative
2. Approximation of Integral

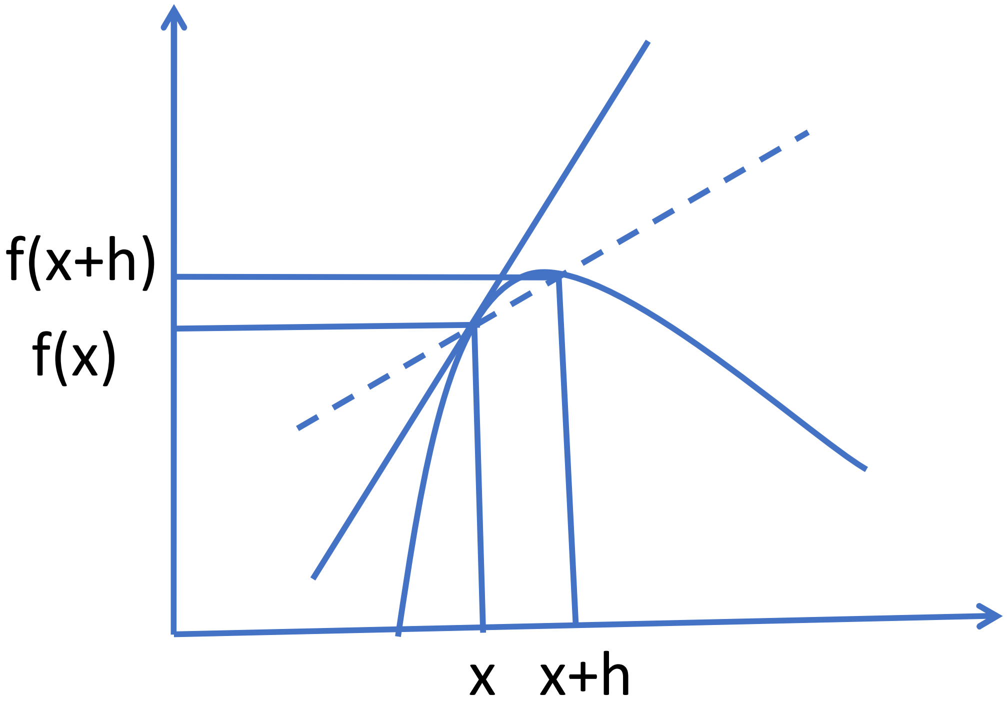
APPROXIMATION OF DERIVATIVE

Derivative Problem

- The first order Derivative :

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

- Geometric meaning:
  - f'(x) is the slope of tangent at point x (solid – line)
- Approximation:
  - $h \neq 0$
  - f'(x) is the slope of secant (dashed – line)



Forward Difference Method (FD)

- Formulate the method: Consider the Taylor expansion of the function f at the neighborhood of x:

$$f(x+h) = f(x) + f^{'}(x)h + f^{''}(\zeta)\frac{h^2}{2!} \qquad (1)$$

where ξ belong to [x,x+h].

From (1) =>:

$$f^{'}(x) = \frac{f(x+h) - f(x)}{h} + f^{''}(\zeta)\frac{h}{2!} \qquad (2)$$

Given that f”(ξ) h/2 is the truncation error, from (2) =>:

$$f^{'}(x) \approx \frac{f(x+h) - f(x)}{h} \qquad (3)$$

(3) is the Forward Difference (FD) formula to approximate the derivative

FD: Error analysis

- Truncation error : f''(ξ) h/2= O(h)

⇒This method has accuracy of first order

- Rounding error: When calculating f(x) and f(x+h), if there is a rounding error, the formula for f':

$$\frac{f(x+h)(1+\delta_1)-f(x)(1+\delta_2)}{h}=\frac{f(x+h)-f(x)}{h}+\frac{\delta_1 f(x+h)-\delta_2 f(x)}{h}$$

Because |δi| is smaller than the accuracy of the computer ε, so the rounding error when calculating f' is:

$$\frac{\varepsilon(|f(x+h)|+|f(x)|)}{h}$$

- The total error is minimal when:

$$h\approx\sqrt{\varepsilon}$$

FD: Example

- Consider the function: $f(x) = \sin(x)$. Use the forward difference method to approximate $f'(\pi/3)$.
- Error analysis
  - Calculate with $h=10^{-k}$, $k = 1,\ldots,16$
  - Find h for minimum error

Result

h	Derivative	Error
10^{-1}	0.455901885410761	-0.044098114589239
10^{-2}	0.495661575773687	-0.004338424226313
10^{-3}	0.499566904000770	-0.000433095999230
10^{-4}	0.499956697895820	-0.000043302104180
10^{-5}	0.499995669867026	-0.000004330132974
10^{-6}	0.499999566971887	-0.000000433028113
10^{-7}	0.499999956993236	-0.000000043006764
10^{-8}	0.499999996961265	-0.000000003038736
10^{-9}	0.500000041370186	0.000000041370185

Backward Difference Method (BD)

- Formulate the method: Similar to the forward difference method, in Taylor expansion we use x-h instead of x+h, we have :

$$f'(x) \approx \frac{f(x) - f(x-h)}{h} \qquad (1)$$

- Error: As same as in forward difference, backward difference has the first order accuracy
  - Minimum error when: $h \approx \sqrt{\varepsilon}$

- Exercise: Use the BD to approximate f'(π/3), knowing that f(x) = sin(x)

Central Difference Method (CD)

- Formulate the method: Consider the Taylor expansion of the function f at the neighborhood x:

$$f(x-h) = f(x) - f'(x)h + f''(x)\frac{h^2}{2!} - f'''(\zeta^-)\frac{h^3}{3!} \qquad (1)$$

$$f(x+h) = f(x) + f'(x)h + f''(x)\frac{h^2}{2!} + f'''(\zeta^+)\frac{h^3}{3!} \qquad (2)$$

where ξ+ belongs to [x,x+h], ξ- belongs to [x-h,x]. From (1) and (2), we have:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \qquad (3)$$

(3) is the Central Difference (CD) method

CD: Error Analysis

- Truncation error:

$$-\frac{1}{6} f'''(\zeta)h^2, \qquad \zeta \in [x-h, x+h]$$

  - CD method has accuracy order of 2;
  - Error minimal when $h = \varepsilon^{1/3}$

- Exercise: Use the CD method to approximate f'(π/3), knowing that f(x) = sin(x). Compare with FD and BD method

Compare error of: FD, BD, CD

h	FD	BD	CC
10^{-1}	$\sim10^{-2}$	$\sim10^{-2}$	$\sim10^{-4}$
10^{-2}	$\sim10^{-3}$	$\sim10^{-3}$	$\sim10^{-6}$
10^{-3}	$\sim10^{-4}$	$\sim10^{-4}$	$\sim10^{-8}$
10^{-4}	$\sim10^{-5}$	$\sim10^{-5}$	$\sim10^{-10}$
10^{-5}	$\sim10^{-6}$	$\sim10^{-6}$	**$\sim10^{-12}$**
10^{-6}	$\sim10^{-7}$	$\sim10^{-7}$	$\sim10^{-11}$
10^{-7}	$\sim10^{-8}$	$\sim10^{-8}$	$\sim10^{-10}$
10^{-8}	**$\sim10^{-9}$**	**$\sim10^{-9}$**	$\sim10^{-9}$
10^{-9}	$\sim10^{-8}$	$\sim10^{-8}$	$\sim10^{-8}$

Approximation of second order derivative

- Consider the Taylor expansion of the function f at the neighborhood x:

$$f(x-h) = f(x) - f'(x)h + f''(h)\frac{h^2}{2!} - f'''(x)\frac{h^3}{3!} + f''''(x)\frac{h^4}{4!} - f'''''(x)\frac{h^5}{5!} + \ldots (1)$$

$$f(x+h) = f(x) + f'(x)h + f''(h)\frac{h^2}{2!} + f'''(x)\frac{h^3}{3!} + f''''(x)\frac{h^4}{4!} + f'''''(x)\frac{h^5}{5!} + \ldots (2)$$

- From (1) and (2), we have the approximate formula for 2nd order derivative

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \qquad (3)$$

- Truncation error:
  - Minimum when h = $\varepsilon^{1/4}$

$$-\frac{1}{12} f''''(\zeta)h^2, \qquad \zeta \in [x-h, x+h]$$

Approximation of partial derivative

- Similarly, we can formulate the approximate formula for partial derivative, for example, central difference for partial derivatives of function f(x,y) as follows:

$$\frac{\partial f(x,y)}{\partial x} = \frac{f(x+h,y) - f(x-h,y)}{2h}$$

$$\frac{\partial f(x,y)}{\partial y} = \frac{f(x,y+h) - f(x,y-h)}{2h}$$

APPROXIMATION OF INTEGRAL

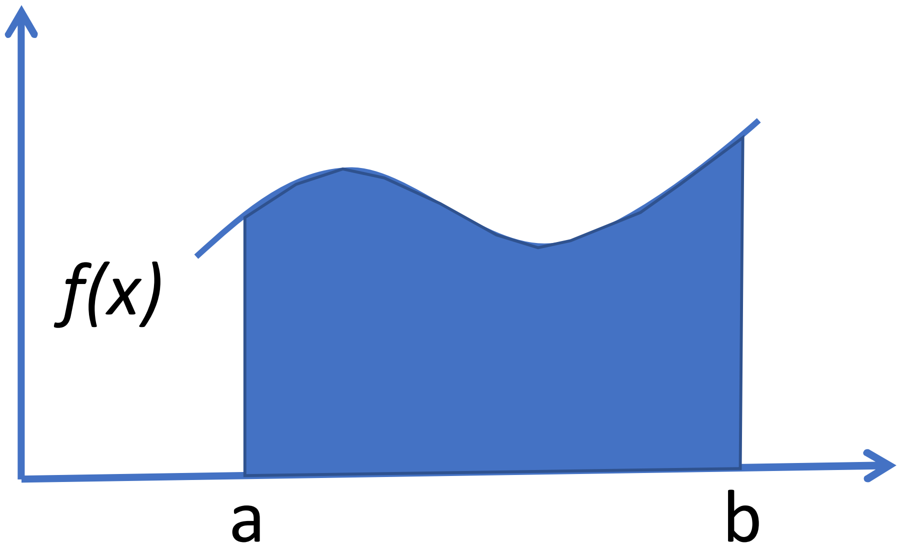
Integral Problem

- Integral formula:

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

where f(x) is an integrable function on the interval [a,b]

- Geometrical meaning:



Riemann Sum

- Suppose the function f defined on [a,b] and Δ is the division of the interval [a,b] into n closed sub-intervals $I_k=[x_{k-1},x_k]$, k=1,…,n, where $a = x_0 < x_1 < \ldots < x_{n-1} < x_n = b$. Choose n points $\{c_k: k=1,\ldots,n\}$, each of which belongs to a sub-interval, that is: c_k belongs to I_k for all k. The sum:

$$\sum_{k=1}^{n} f(c_k)\Delta x_k = f(c_1)\Delta x_1 + f(c_2)\Delta x_2 + \ldots + f(c_n)\Delta x_n$$

is called the Riemann sum of the function f(x) corresponding to the division Δ and the selection points $\{c_k: k=1,\ldots,n\}$.

Approximating Integral

- The definite integral of the function f(x) wrt x from a to b is the limit of the Riemann sum

$$\int_a^b f(x)dx = \lim_{n \to \infty} \sum_{k=1}^{n} f(c_k)\Delta x_k ,$$

- It is assumed that this limit exists.
    - The function f(x) is called the function to be integrated
    - a, b are the integral limitations
    - [a,b] is the integral interval

Properties of definite integrals

$$\int_a^a f(x)\,dx = 0$$

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

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

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

$$\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx, \qquad c \in [a, b]$$

Theorems

- Theorem 1: If f is continuous on [a,b] and F is a primitive of the function f (F' = f), then:

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

- Theorem 2 (Theorem about mean value): If f is continuous on [a,b], there exists a number c in the interval [a,b] such that :

$$f(c) = \frac{1}{b-a}\int_a^b f(x)dx$$

Newton-Cotes formula

- The first approach to formulate an integral approximation is to approximate the function f(x) over the integral interval [a,b] by a polynomial. In each subinterval we approximate the function f(x) by a polynomial:

$$p_m(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_m x^m \qquad (1)$$

- We can replace the function f(x) by an interpolated polynomial (1).
- And then easily calculate the exact integral of interpolated polynomial

Newton-Cotes formula

- Replace f(x) with Lagrange interpolated polynomial, we have:

$$\int_a^b f(x)dx = \int_b^a \left(\sum_{i=0}^{m} \prod_{\substack{j=0 \\ j\neq i}}^{m} \frac{x - x_j}{x_i - x_j} f(x_i) \right) dx$$

$$= \sum_{i=0}^{m} f(x_i) \int_a^b \prod_{\substack{j=0 \\ j\neq i}}^{m} \frac{x - x_j}{x_i - x_j} dx \qquad (1)$$

Newton-Cotes formula

- Error of the method is evaluated by:

$$\int_a^b f(x)dx - \int_a^b p_m(x)dx = \frac{1}{(m+1)!}\int_b^a f^{(m+1)}(\zeta_x)\left(\prod_{i=0}^{m}(x-x_i)\right)dx$$

$$\zeta_x \in [a,b] \qquad (2)$$

Newton-Cotes formula

- The integral approximation formulas are obtained with this approach which uses an equal grid in the integral interval, i.e.:

$$x_i = a+i*h;\ i=0,1,\ldots,m;\ h=(b-a)/m,$$

is called the Newton-Cotes formula.

- For different m, we have different Newton-Cotes formulas

m	Order	Formula	Error
1	1	Trapezoidal rule	$O(h^2)$
2	2	Simpson 1/3	$O(h^4)$
3	3	Simpson 3/8	$O(h^4)$

Trapezoidal rule

- For n=1, the interpolated polynomial has the form:

$$p_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

$$\Rightarrow I = \int_a^b f(x)dx \approx \int_a^b p_1(x)dx = \int_a^b \left(f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right) dx$$

$$\Rightarrow I = \frac{\left(f(a) + f(b)\right)}{2}(b - a) \qquad (1)$$

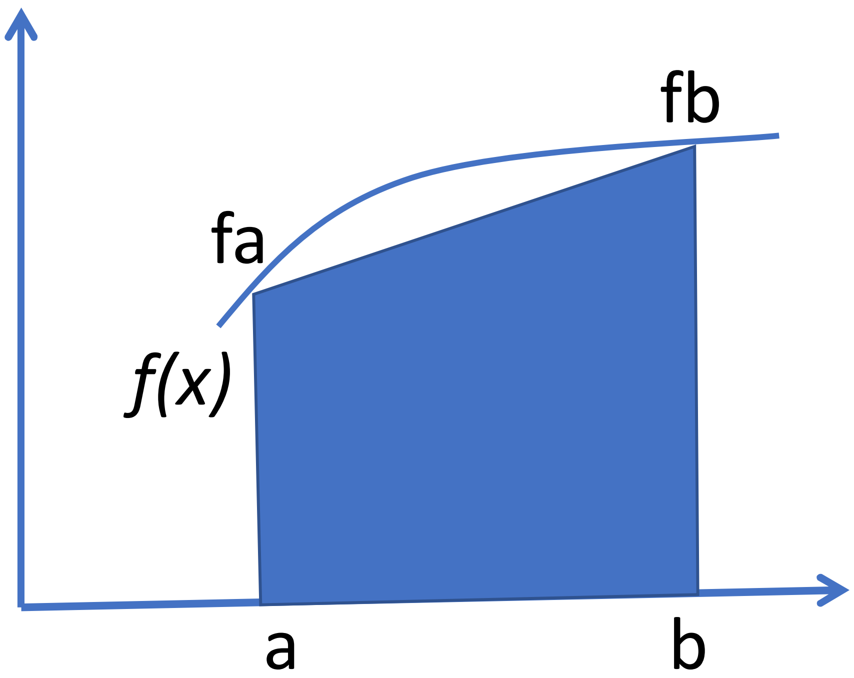
- (1) is called the Trapezoidal formula for approximating the integral

Trapezoidal rule

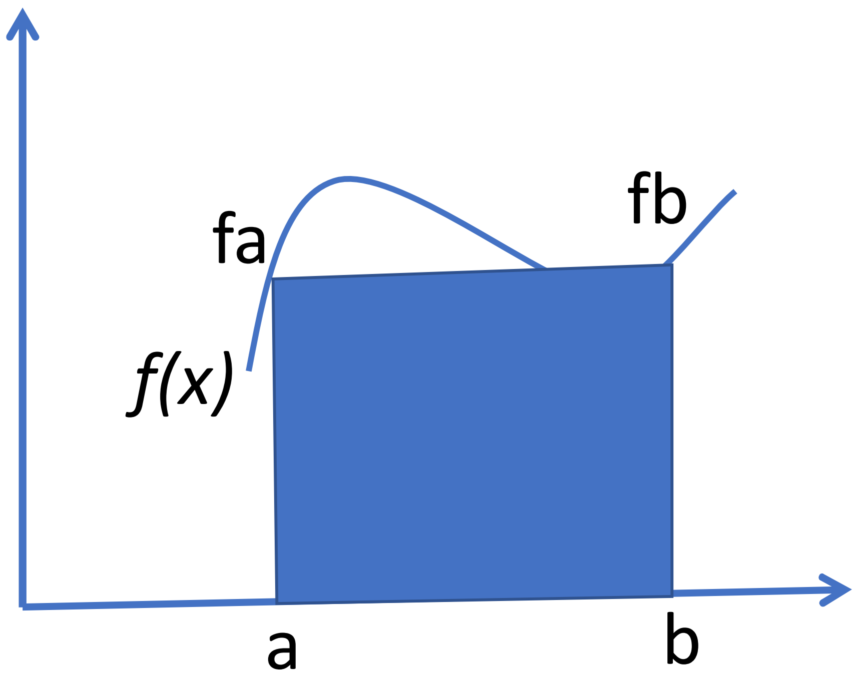
- Error of trapezoidal rule:

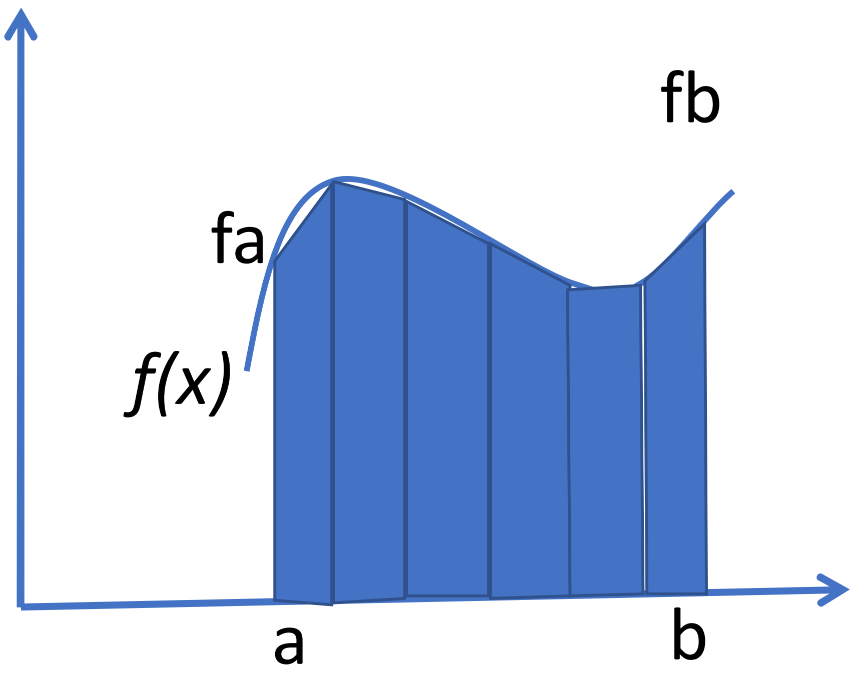
$$-\frac{b-a}{12} f''(\zeta)h^2, \qquad h = b-a, \quad \zeta \in [a,b]$$

- Geometrical meaning:



Trapezoidal rule: Extension





- The idea of the extended trapezoidal formula: Divide the interval [a,b] into subintervals in order to reduce the error

Trapezoidal rule: Extension

- Divide [a,b] into n equal intervals using n+1 points:

$x_0 = a,\ x_1 = a + h,\ x_{n-1} = a + (n-1)*h,\ x_n = a + n*h$

where h = (b-a)/n, we have:

$$I = \int_a^b f(x)dx = \int_a^{a+h} f(x)dx + \int_{a+h}^{a+2h} f(x)dx + \ldots + \int_{a+(n-1)h}^{a+nh} f(x)dx \qquad (1)$$

- Applying the trapezoidal formula for each subinterval we have:

$$I = \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f(a+ih) + f(b) \right] \qquad (2)$$

- (2) is called the expanded trapezoid formula

Simpson 1/3 formula

- Substituting n=2 into the Newton-Cotes formula and integrating, we get:

$$I = \int_a^b f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

$$x_0 = a, \qquad x_1 = a + h, \qquad x_2 = a + 2h = b, \qquad (1)$$

- (1) is called Simpson's formula 1/3

Simpson 1/3 formula: Extension

- Like the extended trapezoidal rule, we divide the interval [a,b] into several subintervals and apply the Simpson 1/3 to each subinterval, we get the extended Simpson 1/3:

$$I = \int_a^b f(x)dx = (b-a)\frac{f(x_0) + 4\sum_{i=1,3,5,..}^{n-1} f(x_i) + 2\sum_{j=2,4,6,..}^{n-2} f(x_j) + f(x_n)}{3n}$$

$$x_0 = a, \quad x_i = a + ih, \quad i = 1,\ldots,n, \quad (1)$$

- Note: We need an even number of subintervals, or an odd number of points.

Simpson 3/8 formula

- Substituting n=3 into the Newton-Cotes formula and integrating, we get:

$$I = \int_a^b f(x)dx = \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]$$

$$x_0 = a, \qquad x_1 = a + h, \qquad x_2 = a + 2h, \qquad x_3 = a + 3h \qquad (1)$$

- (1) is called Simpson formula 3/8

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