Computational Physics

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Lecture-07

Contents

- Basis Concepts
- Numerical Differentiation
- Numerical Integration

Numerical Integration

- Gaussian Quadrature Rule

One-point: $$\int_a^b f(x)\mathrm{d}x \approx C_1 f(x_1)$$

Two-point: $$\int_a^b f(x)\mathrm{d}x \approx C_1 f(x_1) + C_2 f(x_2)$$

$$\vdots$$

n-point: $$\int_a^b f(x)\mathrm{d}x \approx C_1 f(x_1) + C_2 f(x_2) + \cdots + C_n f(x_n)$$

Numerical Integration

- Gaussian Quadrature Rule

One-point (Midpoint)

$$\int_a^b f(x)\mathrm{d}x \approx C_1 f(x_1), \qquad C_1, x_1 = ?, \qquad a \le x_1 \le b$$

A linear choice: $f(x) = a_0 + a_1 x, \qquad$ arbitrary a_0 and a_1

Left Side: $\int_a^b f(x)\mathrm{d}x = \int_a^b (a_0 + a_1 x)\mathrm{d}x = a_0(b-a) + a_1 \frac{(b^2 - a^2)}{2}$

Right Side: $C_1 f(x_1) = C_1(a_0 + a_1 x_1) = a_0(C_1) + a_1(C_1 x_1)$

Numerical Integration

- Gaussian Quadrature Rule

One-point (Midpoint)

$$\int_a^b f(x)\mathrm{d}x \approx C_1 f(x_1), \qquad C_1, x_1 = ?, \qquad a \leq x_1 \leq b$$

Left Side: $$\int_a^b f(x)\mathrm{d}x = a_0(b-a) + a_1 \frac{(b^2-a^2)}{2}$$

Right Side: $$C_1 f(x_1) = a_0(C_1) + a_1(C_1 x_1)$$

$$\Longrightarrow \begin{cases} C_1 = b - a \\ C_1 x_1 = \dfrac{b^2 - a^2}{2} \end{cases}$$

$$C_1 = b - a, \quad x_1 = \frac{b+a}{2} \Longrightarrow \boxed{\int_a^b f(x)\mathrm{d}x \approx (b-a) f(\frac{b+a}{2})}$$

Numerical Integration

- Gaussian Quadrature Rule

One-point (Midpoint)

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)f(\frac{b+a}{2})$$

A linear choice: $f(x) = a_0 + a_1 x,$ arbitrary a_0 and a_1

$$f(\frac{b+a}{2}) = a_0 + a_1\frac{b+a}{2} = \left(\frac{a_0}{2} + \frac{a_1}{2}b\right) + \left(\frac{a_0}{2} + \frac{a_1}{2}a\right) = \frac{f(a)+f(b)}{2}$$

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)\frac{f(a)+f(b)}{2}$$

$\Longrightarrow$ Midpoint is equivalent with Trapezoidal

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_a^b f(x)\mathrm{d}x \approx C_1 f(x_1) + C_2 f(x_2), \quad C_1, C_2, x_1, x_2 \; = ?, \quad a \le x_1, x_2 \le b$$

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3, \qquad \text{arbitrary } a_0, a_1, a_2 \text{ and } a_3$$

Left Side: $\displaystyle\int_a^b f(x)\mathrm{d}x = a_0(b-a) + a_1\frac{(b^2-a^2)}{2} + a_2\frac{(b^3-a^3)}{3} + a_3\frac{(b^4-a^4)}{4}$

Right Side: $C_1 f(x_1) + C_2 f(x_2) = a_0(C_1 + C_2) + a_1(C_1 x_1 + C_2 x_2)$

$$+a_2(C_1 x_1^2 + C_2 x_2^2) + a_3(C_1 x_1^3 + C_2 x_2^3)$$

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_a^b f(x)\mathrm{d}x \approx C_1 f(x_1) + C_2 f(x_2), \quad C_1, C_2, x_1, x_2 = ?, \quad a \leq x_1, x_2 \leq b$$

$$\begin{cases} C_1 + C_2 = b - a \\ C_1 x_1 + C_2 x_2 = \dfrac{b^2 - a^2}{2} \\ C_1 x_1^2 + C_2 x_2^2 = \dfrac{b^3 - a^3}{3} \\ C_1 x_1^3 + C_2 x_2^3 = \dfrac{b^4 - a^4}{4} \end{cases}$$

- □ Four Nonlinear equations
- □ Four unknown variables

Hard to Solve!

Numerical Integration

- Gaussian Quadrature Rule

Two-point

Easy way to Solve!

$$\int_a^b f(x)\mathrm{d}x$$

$$x = \frac{b+a}{2} + \frac{b-a}{2}s : \quad \mathrm{d}x = \frac{b-a}{2}\mathrm{d}s, \quad s=-1 \Rightarrow x=a, \quad s=1 \Rightarrow x=b$$

$$\int_a^b f(x)\mathrm{d}x = \frac{b-a}{2}\int_{-1}^{1} f(\frac{b+a}{2} + \frac{b-a}{2}s)\mathrm{d}s = \frac{b-a}{2}\int_{-1}^{1} g(s)\mathrm{d}s$$

$$f(\frac{b+a}{2} + \frac{b-a}{2}s) = g(s) : \quad \int_{-1}^{1} g(s)\mathrm{d}s$$

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_{-1}^{1} g(s)\mathrm{d}s \approx C_1 g(s_1) + C_2 g(s_2), \quad C_1, C_2, s_1, s_2 = ?, \quad -1 \leq s_1, s_2 \leq 1$$

$$g(s) = a_0 + a_1 s + a_2 s^2 + a_3 s^3, \qquad \text{arbitrary } a_0, a_1, a_2 \text{ and } a_3$$

$$\text{Left Side: } \int_{-1}^{1} g(s)\mathrm{d}s = 2a_0 + 0a_1 + \frac{2}{3}a_2 + 0a_3$$

$$\text{Right Side: } C_1 g(s_1) + C_2 g(s_2) = a_0(C_1 + C_2) + a_1(C_1 s_1 + C_2 s_2)$$
$$+ a_2(C_1 s_1^2 + C_2 s_2^2) + a_3(C_1 s_1^3 + C_2 s_2^3)$$

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_{-1}^{1} g(s)\mathrm{d}s \approx C_1 g(s_1) + C_2 g(s_2), \quad C_1, C_2, s_1, s_2 = ?, \quad -1 \leq s_1, s_2 \leq 1$$

$$\begin{cases} C_1 + C_2 = 2 \\ C_1 s_1 + C_2 s_2 = 0 \\ C_1 s_1^2 + C_2 s_2^2 = \dfrac{2}{3} \\ C_1 s_1^3 + C_2 s_2^3 = 0 \end{cases}$$

$$s_1^2 \begin{cases} C_1 s_1 + C_2 s_2 = 0 \\ C_1 s_1^3 + C_2 s_2^3 = 0 \end{cases} \Rightarrow \begin{cases} C_1 s_1^3 + C_2 s_2 s_1^2 = 0 \\ C_1 s_1^3 + C_2 s_2^3 = 0 \end{cases}$$

$$C_2 s_2 (s_2^2 - s_1^2) = 0$$

$$\Downarrow$$

$$C_2 = 0,\ s_2 = 0,\ s_2 = s_1,\ s_2 = -s_1$$

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_{-1}^{1} g(s)\mathrm{d}s \approx C_1 g(s_1) + C_2 g(s_2), \quad C_1, C_2, s_1, s_2 = ?, \quad -1 \le s_1, s_2 \le 1$$

$$\begin{cases} C_1 + C_2 = 2 \\ C_1 s_1 + C_2 s_2 = 0 \\ C_1 s_1^2 + C_2 s_2^2 = \dfrac{2}{3} \\ C_1 s_1^3 + C_2 s_2^3 = 0 \end{cases}$$

$$\begin{cases} \underline{C_2 = 0}: \\ C_1 s_1 + C_2 s_2 = 0 \\ C_1 s_1^2 + C_2 s_2^2 = \dfrac{2}{3} \end{cases} \Longrightarrow \begin{cases} C_1 s_1 = 0 \\ C_1 s_1^2 = \dfrac{2}{3} \end{cases}$$

$C_2 = 0$ is not acceptable.

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_{-1}^{1} g(s)\mathrm{d}s \approx C_1 g(s_1) + C_2 g(s_2), \quad C_1, C_2, s_1, s_2 = ?, \quad -1 \le s_1, s_2 \le 1$$

$$\begin{cases} C_1 + C_2 = 2 \\ C_1 s_1 + C_2 s_2 = 0 \\ C_1 s_1^2 + C_2 s_2^2 = \dfrac{2}{3} \\ C_1 s_1^3 + C_2 s_2^3 = 0 \end{cases}$$

$$\begin{cases} \underline{s_2 = 0:} \\ C_1 s_1 + C_2 s_2 = 0 \\ C_1 s_1^2 + C_2 s_2^2 = \dfrac{2}{3} \end{cases} \Longrightarrow \begin{cases} C_1 s_1 = 0 \\ C_1 s_1^2 = \dfrac{2}{3} \end{cases}$$

$s_2 = 0$ is not acceptable.

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_{-1}^{1} g(s)\mathrm{d}s \approx C_1 g(s_1) + C_2 g(s_2), \quad C_1, C_2, s_1, s_2 = ?, \quad -1 \leq s_1, s_2 \leq 1$$

$$\begin{cases} C_1 + C_2 = 2 \\ C_1 s_1 + C_2 s_2 = 0 \\ C_1 s_1^2 + C_2 s_2^2 = \dfrac{2}{3} \\ C_1 s_1^3 + C_2 s_2^3 = 0 \end{cases} \qquad \begin{cases} \underline{s_2 = s_1} : \\ C_1 + C_2 = 2 \\ s_1(C_1 + C_2) = 0 \\ s_1^2(C_1 + C_2) = \dfrac{2}{3} \end{cases}$$

$s_2 = s_1$ is not acceptable.

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_{-1}^{1} g(s)\mathrm{d}s \approx C_1 g(s_1) + C_2 g(s_2), \quad C_1, C_2, s_1, s_2 = ?, \quad -1 \le s_1, s_2 \le 1$$

$$\begin{cases} C_1 + C_2 = 2 \\ C_1 s_1 + C_2 s_2 = 0 \\ C_1 s_1^2 + C_2 s_2^2 = \dfrac{2}{3} \\ C_1 s_1^3 + C_2 s_2^3 = 0 \end{cases} \qquad \begin{cases} \underline{s_2 = -s_1} : \\ \left. \begin{array}{l} C_1 + C_2 = 2 \\ s_1^2 (C_1 + C_2) = \dfrac{2}{3} \end{array} \right\} \Longrightarrow \begin{cases} s_1 = \pm \dfrac{1}{\sqrt{3}} \\ s_2 = \mp \dfrac{1}{\sqrt{3}} \\ C_1 = C_2 = 1 \end{cases} \\ s_1 (C_1 - C_2) = 0 \end{cases}$$

$s_2 = -s_1$ is acceptable.

Numerical Integration

- Gaussian Quadrature Rule

Two-point

$$\int_{-1}^{1} g(s)\mathrm{d}s \approx C_1 g(s_1) + C_2 g(s_2), \quad C_1, C_2, s_1, s_2 = ?, \quad -1 \leq s_1, s_2 \leq 1$$

$$s_1 = -\frac{1}{\sqrt{3}}, \quad s_2 = \frac{1}{\sqrt{3}}, \quad C_1 = C_2 = 1$$

$$\int_{a}^{b} f(x)\mathrm{d}x \approx \frac{b-a}{2}(C_1 f(x_1) + C_2 f(x_2))$$

$$x_1 = \frac{b+a}{2} - \frac{1}{\sqrt{3}}\frac{b-a}{2}, \quad x_2 = \frac{b+a}{2} + \frac{1}{\sqrt{3}}\frac{b-a}{2}, \quad C_1 = C_2 = 1$$

Numerical Integration

- Gaussian Quadrature Rule

$$\int_{-1}^{1} g(s)\mathrm{d}s \approx \sum_{i=1}^{n} C_i g(s_i)$$

Arguments and weights in table

points	arguments	weights
1	0	2
2	$-1/\sqrt{3}$	1
	$1/\sqrt{3}$	1
3	$-\sqrt{3/5}$	$5/9$
	0	$8/9$
	$\sqrt{3/5}$	$5/9$
$\vdots$	$\vdots$	$\vdots$