Differentiation and Integration Lecture Notes

BM 531
Numerical Methods and C/C++ Programming

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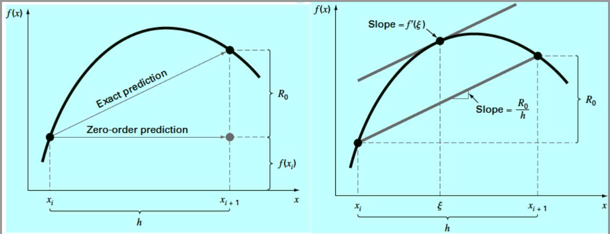
Numerical Differentiation

Forward Difference Formula

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{h}{2} f''(\xi)$$



$$R_0 = f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \dots$$
$$R_0 \approx f'(x_i)h$$

$$R_0 = f'(\xi)h$$

$$R_1 = \frac{f''(x_i)}{2!}h^2 + \dots$$
$$R_1 \approx \frac{f''(x_i)}{2!}h^2$$

$$R_1 = \frac{f''(\xi)}{2!}h^2$$

Central Difference Formula

$$f'(x_i) \approx \frac{f(x_{i+1}) - 2f(x) + f(x_{i-1})}{2h}$$

$$f'(x_i) = \frac{f(x_{i+1}) - 2f(x) + f(x_{i-1})}{2h} + E_{trunc}(f, h)$$

where $E_{trunc}(f, h) = -\frac{h^2 f^3(c)}{3!} = O(h^2)$ is the truncation error.

Proof:

From Taylor Series Expansion of $f(x+h)$ and $f(x-h)$

$$f(x+h) - f(x-h) \approx 2f'(x)h + \frac{[f^{(3)}(c_1) + f^{(3)}(c_2)]}{3!}$$

$$f^{(3)}(c) = \frac{f^{(3)}(c_1) + f^{(3)}(c_2)}{2}$$

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} - \frac{f^{(3)}(c)h^2}{3!}$$

The Centered Formula of Order $O(h^4)$

$$f'(x) = \frac{-f(x+2h)+8f(x+2h)-8f(x-h)+f(x-2h)}{12h} + E_{trunc}(f,h)$$

$E_{trunc}(f,h) = \frac{h^4 f^5(c)}{30} = O(h^4)$ is called the truncation error.

Proof:

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{2f^{(3)}(x)h^3}{3!} + \frac{2f^{(5)}(c_1)h^5}{5!}$$

$$f(x+2h) - f(x-2h) = 4f'(x)h + \frac{16f^{(3)}(x)h^3}{3!} + \frac{64f^{(5)}(c_2)h^5}{5!}$$

By eliminating $f^{(3)}$

$$-f(x+2h) + f(x+h) - 8f(x-h) + f(x-2h) =$$
$$12f'(x)h + (16f^{(5)(c_1)} - 64f^{(5)}(c_2))h^{5/120}$$

$$f'(x) = \frac{-f(x+2h)+f(x+h)-8f(x-h)+f(x-2h)}{12h} + \frac{f^{(5)}(c)h^4}{30}$$

Error Analysis

$f'(x) \approx \frac{-y_2+8y_1-8y_{-1}+y_{-2}}{12h}$ where $y_i = f(x+ih)$

$$E(f,h) = E_{round}(f,h) + E_{trunc}(f,h)$$

$$|E(f,h)| \le \frac{3\epsilon}{2h} + \frac{Mh^4}{30}$$

3^{rd} Order Lagrange Formulation of Numerical Differentiation

$$f(x) = f(x_0)\frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)} +$$
$$f(x_1)\frac{(x-x_0)(x-x_2)(x-x_3)(x-x_4)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)(x_1-x_4)} + f(x_2)\frac{(x-x_0)(x-x_1)(x-x_3)(x-x_4)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)(x_2-x_4)} +$$
$$f(x_3)\frac{(x-x_0)(x-x_1)(x-x_2)(x-x_4)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)(x_3-x_4)} + f(x_4)\frac{(x-x_0)(x-x_1)(x-x_2)(x-x_3)}{(x_4-x_0)(x_4-x_1)(x_4-x_2)(x_4-x_3)}$$

$$\int_{x_0}^{x_2} f(x)dx \approx f(x_0)\int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}dx +$$
$$f(x_1)\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}dx + f(x_2)\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx$$

$x = x_0 + ht$ with $dx = hdt$ $x_j = x_0 + hj$ $x_j - x_k = h(j-k)$ and $x - x_j = h(t-j)$

$$f^{(3)}(t) \approx f_0\frac{6[(t-x_1)+(t-x_2)+(t-x_3)+(t-x_4)]}{(-h)(-2h)(-3h)(-4h)}$$
$$+f_1\frac{6[(t-x_0)+(t-x_2)+(t-x_3)+(t-x_4)]}{(h)(-h)(-3h)(-4h)}$$
$$+f_2\frac{6[(t-x_0)+(t-x_1)+(t-x_3)+(t-x_4)]}{(2h)(-h)(-h)(-2h)} + f_3\frac{6[(t-x_0)+(t-x_1)+(t-x_2)+(t-x_4)]}{(3h)(2h)(h)(-h)}$$
$$+f_4\frac{6[(t-x_0)+(t-x_1)+(t-x_2)+(t-x_3)]}{(4h)(3h)(2h)(h)}$$

When $t = x_0$ and $t - x_j = x_0 - x_j = -jh$

$$f^{(3)}(x_0) \approx \frac{-5f_0+18f_1-24f_2+14f_3-3f_4}{2h^3}$$

Numerical Integration

Introduction to Quadrature

$a = x_0 < x_1 < \ldots < x_m = b$

$Q[f] = \sum_{j=0}^{M} w_j f(x_j) = w_0 f(x_0) + w_1 f(x1) + \ldots + w_M f(x_M)$

$\int_a^b f(x)dx = Q[f] + E[f]$

Trapezoidal Rule:

Trapezodial Rule has a degree of precision with $n = 1$.

$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12} f^{(2)}(c)$

Using 2^{nd} order Lagrange Interpolation to $f(x)$

$f(x) \approx f(x_i)\frac{(x-x_{i+1})}{(x_i-x_{i+1})} + f(x_{i+1})\frac{(x-x_i)}{(x_{i+1}-x_i)}$

$\int_{x_i}^{x_{i+1}} f(x)dx \approx (x_{i+1} - x_i)[\frac{f(x_i)+f(x_{i+1}))}{2}]$

$x_a = x_0, x_1, \ldots, x_N = x_b$ with N number of intervals with $\Delta x = x_{i+1} - x_i$ width.

$\int_{x_a}^{x_b} f(x)dx \approx \sum_{i=0}^{N-1}[\int_{x_i}^{x_{i+1}} f(x)dx]$

$I = \frac{\Delta x}{2}[f(x_0 + f(x_N))] + \Delta x[f(x_1) + \ldots + f(x_{n-1})]$

Iterative Algorithm

$x_{2m-1} = x_a + [2m-1]\Delta x_r \;\; m = 1, 2, \ldots, k$

$\Delta x_r = \Delta x_{r-1}/2$ with $k = 2^{r-1}$ new control points

$I_r = I_{r-1} + \Delta x_r[f(x_1) + f(x_2) + \ldots + f(x_{2k-1})]$

Simpson's Rule has a degree of precision with $n = 3$.

$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90}f^{(4)}(c)$

Proof for Simpson's Rule:

Using 2^{nd}order Lagrange interpolator

$$f(x) = f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

$$\int_{x_0}^{x_2} f(x)dx \approx f(x_0)\int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}dx + f(x_1)\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}dx + f(x_2)\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx$$

$x = x_0 + ht$ with $dx = hdt$ $x_j = x_0 + hj$ $x_j - x_k = h(j-k)$ and $x - x_j = h(t-j)$

$$\int_{x_0}^{x_2} f(x)dx \approx f_0\int_0^2 \frac{(h)(t-1)(h)(t-2)}{(-h)(-2h)}hdt + f_1\int_0^2 \frac{(h)(t-0)(h)(t-2)}{(h)(-h)}hdt + f_2\int_0^2 \frac{(h)(t-0)(h)(t-1)}{(2h)(h)}hdt = \frac{h}{3}(f_0 + 4f_1 + f_2)$$

$x_a = x_0, x_1, \ldots, x_{2N} = x_b$ with $2N$ number of intervals with $\Delta x = x_{i+1} - x_i$ width.

$$\int_{x_a}^{x_b} f(x)dx \approx \sum_{i=0}^{N-1}[\int_{x_{2i}}^{x_{(2i+2)}} f(x)dx]$$

$$\approx \sum_{i=0}^{N-1}[x_{2i+2} - x_{2i}][f(x_{2i} + 4f(x_{2i+1}) + f(x_{2i+2})]/6$$

$(I_s)_{2j} = (4/3)(I_t)_{2j} - (1/3)(I_t)_j$

$(I_t)_j$: Trapezoidal rule approximation with $2j$ intervals of Δx size.

$(I_t)_j$: Trapezoidal rule approximation with j intervals of $2\Delta x$ size.

Simpson's $\frac{3}{8}$ Rule results from 3rd order Lagrange Interpolation

$$\int_{x_i}^{x_{i+3}} f(x)dx \approx [x_{i+2} - x_i][f(x_i + 3f(x_{i+1}) + 3f(x_{i+2}) + f(x_{i+3})]/6$$

Simpson's $\frac{3}{8}$ Rule has a degree of precision with $n = 3$.

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80} f^{(4)}(c)$$

Degree of Precision of the Simpson's $\frac{3}{8}$ Rule

$\int_0^3 1dx = 3 = \frac{3}{8}(1 + 3 \times 1 + 3 \times 1 + 1)$

$\int_0^3 xdx = \frac{3}{2} = \frac{3}{8}(0 + 3 \times 1 + 3 \times 2 + 3)$

$\int_0^3 x^2 dx = 9 = \frac{3}{8}(0 + 3 \times 1 + 3 \times 4 + 9)$

$\int_0^3 x^3 dx = \frac{81}{4} = \frac{3}{8}(0 + 3 \times 1 + 3 \times 8 + 27)$

Gauss-Legendre Integration

$y = f(x)$

2-point Rule:

$\int_{-1}^{1} f(x)dx \approx w_1 f(x_1) + w_2 f(x_2)$

$\int_{-1}^{1} 1dx = 2 = w_1 + w_2$

$\int_{-1}^{1} xdx = 0 = w_1 x_1 + w_2 x_2$

$\int_{-1}^{1} x^2 dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2$

$\int_{-1}^{1} x^3 dx = 0 = w_1 x_1^3 + w_2 x_2^3$

Solution set is $-x_1 = x_2 = 1/\sqrt{3}$ and $w_1 = w_2 = 1$

3-point Rule:

$\int_{-1}^{1} f(x)dx \approx \frac{5f(-\sqrt{3/5})+8f(0)+5f(\sqrt{3/5})}{9}$

Gauss-Legendre Translation

Suppose the abscissas $\{x_{n,k}\}_{k=1}^{n}$ and weights $\{w_{n,k}\}_{k=1}^{n}$ are given for n-Point Gauss-Legendre rule over $[-1,1]$.

To apply the rule over $[a,b]$

$t = \frac{a+b}{2} + \frac{b-a}{2}x$ and $dt = \frac{b-a}{2}dx$

$\int_a^b f(t)dt = \int_{-1}^{1} f(\,(a+b)/2 + (b-a)x/2\,)(b-a)dx/2$

$\int_a^b f(t)dt = \int_{-1}^{1} (b-a)/2 \sum_{k=1}^{n} w_{n,k} f(\,(a+b)/2 + (b-a)x_{n,k}/2\,)\,dx$

Gauss-Legendre Quadrature of order n is exact for a function formed by a polynomial of order up to a degree of $2n+2$.

3rd degree

$$\int_{-1}^{1} x^k dx = w_0 x_0^k + w_1 x_1^k = \begin{cases} 0 & k = odd \\ 2/(k+1) & k = even \end{cases} \quad k = 0,1,2,3$$

$w_0 = w_1 = 1$ and $-x_0 = x_1 = 1/\sqrt{3}$

In general, control points x_i are determined by the roots of Legendre polynomials

$P_0(x) = 1,\ P_1(x) = x,$

$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$

with weights $w_i = 2(1 - x_i^2)/((n+1)P_n(x_i))^2$

One point Quadrature $(n = 0)$

$x_0 = 0,\ w_0 = 2$

Two-point Quadrature $(n = 1)$

$-x_0 = x_1 = 1/\sqrt{3}$ and $w_0 = w_1 = 1$

Three-point Quadrature $(n = 2)$

$-x_0 = x_2 = \sqrt{0.6},\ x_1 = 0,\ w_0 = w_2 = 5/9$ and $w_1 = 8/9$

Example

$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$

$\int_0^{0.8} f(x)dx = 1.6405334$

By a change of variables $y = \alpha x + \beta$

$\alpha = 2.5$ and $\beta = 1$

Substitute $x = 0.4y + 0.4$ in $f(x)$

$\int_{-1}^{1} g(y)dy = w_0 x_0 + w_1 x_1 = 1.8225778$

Relative Error $= -11.1\%$