BM 593 Numerical Methods & C Programming

6th week

Numerical Differentiation

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

The Central Difference Formula

$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}$

There exists a number $c = c(x) \in [a, b]$ so that

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

where

$E_{trunc}(f, h) = -\frac{h^2 f^3(c)}{6} = O(h^2)$ is called the truncation error.

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

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

$\frac{[f^{(3)}(c_1)+f^{(3)}(c_2)]}{3!} = f^{(3)}(c)$

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.

Error Analysis

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

$E(f, h) = E_{round}(f, h) + E_{trunc}(f, h) = f'(x) \approx \frac{-e_2+8e_1-8e_{-1}+e_{-2}}{12h} + \frac{h^4 f^{(5)}(c)}{30}$

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

where $|e_k| = \epsilon$ and $M = max_{a \leq x \leq b}\{|f^{(5)}(x)|\}$

$h = \frac{45\epsilon^{1/5}}{4M}$

Lagrange Formulation of Numerical Differentiation

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

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 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:

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

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

$x = x_0 + ht$ 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

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

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

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

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

Gauss-Legendre Integration

$y = f(x)$

2-point Rule:

$\int_{-1}^1 f(x)dx \approx w_1f(x_1) + w_2f(x_2)$

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

$\int_{-1}^1 xdx = 0 = w_1x_1 + w_2x_2$

$\int_{-1}^1 x^2dx = \frac{2}{3} = w_1x_1^2 + w_2x_2^2$

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

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 $[a,b]$

$t = (a+b)/2 + (a-b)x/2$ and $dt = (b-a)dx/2$

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

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

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

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

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

Control Points x_i are determined by the Legendre Polynomials

$P_0(x) = 1,\ P_1(x) = x,\ P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)/(n+1)$

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 $= -11.1\%$