

Chap 4 数值积分和微分

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数值微分

- 前向差分: $f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2} f''(\xi)$, 在 x_0 点误差为 $O(h)$.

- (n+1)-点公式(拉格朗日)

- 三点公式

$$f'(x) = f(x_0) \frac{(2x - x_1 - x_2)}{2h^2} - f(x_1) \frac{(2x - x_0 - x_2)}{h^2} + f(x_2) \frac{(2x - x_1 - x_0)}{2h^2}$$

$$E(x_0) = E(x_2) = \frac{h^2}{3} f^{(3)}(\xi), E(x_1) = \frac{h^2}{6} f^{(3)}(\xi)$$

- 五点公式

- $f'(x_0) = \frac{1}{12h} [f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30} f^{(5)}(\xi),$

系数(1, -8, 8, -1), $O(h^4)$

$$f'(x_0) = \frac{1}{12h} [-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h)$$

$$+ 16f(x_0+3h) - 3f(x_0+4h)] + \frac{h^4}{5} f^{(5)}(\xi),$$

系数(-25, 48, -36, 16, -3)

- 二阶导数中点公式

- $f''(x_0) = \frac{1}{h^2} [f(x_0-h) - 2f(x_0) + f(x_0+h)] - \frac{h^2}{12} f^{(4)}(\xi),$

- 舍入误差

- 以拉氏多项式为例

The total error in the approximation,

$$f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} = \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1),$$

is due both to round-off error, the first part, and to truncation error. If we assume that the round-off errors $e(x_0 \pm h)$ are bounded by some number $\varepsilon > 0$ and that the third derivative of f is bounded by a number $M > 0$, then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M.$$

- 理查森外推

- 用低精度的步长组合出高精度的微分

- $M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \dots$

- 可以用作精简拉氏多项式的计算过程

数值积分

- 求积法(Quadrature), 基于插值多项式。

- Trapezoidal rule (梯形法则) :

$$\int_a^b f(x) dx = \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi)$$

当二阶导恒零时无误差。

- Simpson's rule:

$$\int_{x_0}^{x_2} f(x) dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi)$$

当四阶导恒为0时无误差。

函数在子区间振荡会降低精度

- 封闭牛顿-柯特斯公式

$$\int_a^b f(x) dx \approx \sum_{i=0}^n a_i f(x_i), \quad a_i = \int_{x_0}^{x_n} \prod_{j=0, j \neq i}^n \frac{x - x_j}{x_i - x_j}$$

- 八分之三法则:

$$\int_{x_0}^{x_3} f(x) dx = \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi)$$

- 只适用小积分区间

- 复合数值积分

- 分段处理

- 复合梯形法则:

$$\int_a^b f(x) dx = \frac{h}{2} \left[f(a) + 2 \sum_{j=1}^{n-1} f(x_j) + f(b) \right] - \frac{b-a}{12} h^2 f''(\mu).$$

- 分成n段后的舍入误差: $e(h) \leq nh\varepsilon$

- Romberg Integration

- 对复合梯形法则应用理查森外推 (误差形式满足理查森外推条件), 取 $n = 1, 2, 4, 8, 16, \dots$

k	$O(h_k^2)$	$O(h_k^4)$	$O(h_k^6)$	$O(h_k^8)$	$O(h_k^{2n})$
1	$R_{1,1}$				
2	$R_{2,1}$	$R_{2,2}$			
3	$R_{3,1}$	$R_{3,2}$	$R_{3,3}$		
4	$R_{4,1}$	$R_{4,2}$	$R_{4,3}$	$R_{4,4}$	
\vdots	\vdots	\vdots	\vdots	\vdots	\ddots
n	$R_{n,1}$	$R_{n,2}$	$R_{n,3}$	$R_{n,4}$	$\dots R_{n,n}$

$$R_{1,1} = \frac{h}{2} (f(a) + f(b)).$$

$$R_{2,1} = \frac{1}{2} \left[R_{1,1} + h \sum_{k=1}^{2^{i-2}} f(a + (k - 0.5)h) \right].$$

$$R_{k,j} = R_{k,j-1} + \frac{1}{4^{j-1} - 1} (R_{k,j-1} - R_{k-1,j-1}), \quad \text{for } k = j, j+1, \dots$$

- 高斯求积法

- 优化牛顿-柯特斯法则的定步长, 使得精度为 $2n-1$ 阶。最小化阶数。

- Legendre多项式

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = x^2 - \frac{1}{3},$$

$$P_3(x) = x^3 - \frac{3}{5}x, \quad \text{and} \quad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}.$$

- 当 $P(x)$ 的阶数小于 $2n$ 时, 令 x_1, x_2, \dots, x_n 是 n 阶勒让德多项式的根, 则

$$c_i = \int_{-1}^1 \prod_{\substack{j=1 \\ j \neq i}}^n \frac{x - x_j}{x_i - x_j} dx.$$

$$\int_{-1}^1 P(x) dx = \sum_{i=1}^n c_i P(x_i).$$