科学计算第六次作业

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Question 0.1. Suppose that $f(x)$ is a smooth function defined on the real line. Let $h > 0$ be a small positive number. Please find a linear combination of $f(x-h)$, $f(x)$ and $f(x+h)$ to approximate the second-order derivative $f''(x)$. That is, find the coefficients α, β and γ so that

$$D_h^2 f(x) \equiv \alpha f(x-h) + \beta f(x) + \gamma f(x+h) \to f''(x) \quad \text{as } h \to 0.$$

Please derive a formula for the approximation error $e_h^2 f(x) = f''(x) - D_h^2 f(x)$ and show the accuracy order of the approximation.

解. 考虑 $\alpha = \frac{1}{h^2}, \beta = -\frac{2}{h^2}, \gamma = \frac{1}{h^2}$, 此时

$$D_h^2 f(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}, \tag{1}$$

在 x 处 Talyor 展开,

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}(\xi_1)}{4!}h^4, \qquad \xi_1 \in (x-h, x), \tag{2}$$

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}(\xi_2)}{4!}h^4, \qquad \xi_2 \in (x, x+h), \tag{3}$$

逼近误差

$$e_h^2 f(x) = \frac{f^{(4)}(\xi_1) + f^{(4)}(\xi_2)}{24}h = \frac{1}{12} f^{(4)}(\xi) h^2, \quad \xi \in (\xi_1, \xi_2). \tag{4}$$

公式具有 3 次代数精度.

Question 0.2. Suppose that $f(x)$ is a smooth function defined on the real line. Let $h > 0$ be a small positive number. Please find a linear combination of $f(x-2h)$, $f(x-h)$, $f(x)$, $f(x+h)$ and $f(x+2h)$ to approximate the second-order derivative$f''(x)$ so that the approximation has fourth-order accuracy.

解. 即找与 h 相关的系数 a_1, a_2, a_3, a_4, a_5 定义

$$D_h^2 f(x) = a_1 f(x-2h) + a_2 f(x-h) + a_3 f(x) + a_4 f(x+h) + a_5 f(x+2h), \tag{5}$$

使得对于 $f(x)$ 为小于等于 4 次的多项式时 $D_h^2 f(x) = f''(x)$ 恒成立, 特别的只要取 $f(x) = 1, x, x^2, x^3, x^4$, 即

$$\begin{aligned}
a_1 \cdot 1 + a_2 \cdot 1 + a_3 \cdot 1 + a_4 \cdot 1 + a_5 \cdot 1 &= 0, \\
a_1 \cdot (x-2h) + a_2 \cdot (x-h) + a_3 \cdot x + a_4 \cdot (x+h) + a_5 \cdot (x+2h) &= 0, \\
a_1 \cdot (x-2h)^2 + a_2 \cdot (x-h)^2 + a_3 \cdot x^2 + a_4 \cdot (x+h)^2 + a_5 \cdot (x+2h)^2 &= 2, \\
a_1 \cdot (x-2h)^3 + a_2 \cdot (x-h)^3 + a_3 \cdot x^3 + a_4 \cdot (x+h)^3 + a_5 \cdot (x+2h)^3 &= 6x, \\
a_1 \cdot (x-2h)^4 + a_2 \cdot (x-h)^4 + a_3 \cdot x^4 + a_4 \cdot (x+h)^4 + a_5 \cdot (x+2h)^4 &= 12x^2,
\end{aligned}$$

化简 (或者代入 $x=0$) 得到

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & 0 & 1 & 2 \\ (-2)^2 & (-1)^2 & 0 & 1^2 & 2^2 \\ (-2)^3 & (-1)^3 & 0 & 1^3 & 2^3 \\ (-2)^4 & (-1)^4 & 0 & 1^4 & 2^4 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \frac{2}{h^2} \\ 0 \\ 0 \end{bmatrix}. \tag{6}$$

解得

$$a_1 = -\frac{1}{12h^2}, \quad a_2 = \frac{4}{3h^2}, \quad a_3 = -\frac{5}{2h^2}, \quad a_4 = \frac{4}{3h^2}, \quad a_5 = -\frac{1}{12h^2}. \tag{7}$$

所以

$$D_h^2 f(x) = \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2}. \tag{8}$$

Question 0.3. Write a C/C++ computer program in double precision to approximately evaluate the first-order derivative of the function $f(x) = e^{-x^2}$ at $x = 1$ with the forward difference $D_h^+ f = \frac{f(x+h) - f(x)}{h}$ and the centered difference $D_h^0 f = \frac{f(x+h) - f(x-h)}{2h}$, respectively. For each numerical difference, choose different parameters $h_k = 10^{-k}$ with the integer $k \in \{1, 2, \cdots, 15\}$ compute the corresponding approximation errors e_{h_k} and make an h_k vs. e_{h_k} plot. Explain on what you observe from the plots.

解. 导函数

$$f'(x) = -2xe^{-x^2}, \tag{9}$$

所以真值为 $f'(1) = -2e^{-1}$.

得到结果

Different Parameters	Forward Errors	Centered Errors
10^{-1}	0.038937264927	0.002454948378
10^{-2}	0.003703013396	0.000024525541
10^{-3}	0.000368124388	0.000000245253
10^{-4}	0.000036790397	0.000000002453
10^{-5}	0.000003678814	0.000000000023
10^{-6}	0.000000367895	-0.000000000005
10^{-7}	0.000000036272	-0.000000000088
10^{-8}	0.000000011847	0.000000003520
10^{-9}	-0.000000071420	-0.000000015909
10^{-10}	-0.000000348976	-0.000000071420
10^{-11}	-0.000002569422	0.000000206136
10^{-12}	-0.000096938379	-0.000041427227
10^{-13}	0.000236128529	-0.000041427227
10^{-14}	-0.002539429033	0.000236128529
10^{-15}	-0.096908386126	-0.041397234895

表 1: Caption

$$(10)$$

Question 0.4. Write a C/C++ computer program to apply the composite trapezoidal rule to evaluate the integral

$$I = \int_0^1 \exp\left\{-\frac{x^2}{2}\right\} \mathrm{d}x \tag{11}$$

by dividing the interval $[0,1]$ into n sub-intervals $\{[x_i, x_{i+1}]\}_{i=0}^{n-1}$ with $x_i = i/n$. For $n = 2, 4, 8, 16, 32$, print out the computed integrals and check the convergence rate (accuracy order) of the solution as n increases. Generate a table as follows. Explain on what you observe.

解. 该积分的真值约为 0.855624.[1] 我们有

$$I_n = \sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2}(x_{i+1} - x_i) = \frac{1}{n}\left(\frac{1 + e^{-\frac{1}{2}}}{2} + \sum_{i=1}^{n-1} e^{-\frac{i^2}{2n^2}}\right), \tag{12}$$

表 2: Computed integrals by the composite trapezodial rule

n	2	4	8	16	32
I_n	0.842881	0.852459	0.854834	0.855427	0.855575
e_n	0.012743	0.003165	0.000790	0.000197	0.000049

...

Question 0.5. Write a C/C++ computer program to apply the composite trapezoidal rule to evaluate the integral

$$I = \int_{-1}^1 (x^2 - 1)^2 \mathrm{d}x, \tag{13}$$

by dividing the interval$[-1, 1]$ into n sub-intervals $\{[x_i, x_{i+1}]\}_{i=0}^{n-1}$ with $x_i = -1 + ih$ and $h = 2/n$. For $n = 2, 4, 8, 16, 32$, print out the computed integrals and check the convergence rate (accuracy order) of the solution as n increases. Explain on what you observe.

解. 本题积分具有解析解

$$I = \int_{-1}^1 x^4 - 2x^2 + 1 \mathrm{d}x = \frac{16}{15}, \tag{14}$$

类似于上一题, 有

$$I_n = \frac{2}{n}\left(\frac{0+0}{2} + \sum_{i=1}^{n-1}\left(\left(-1 + \frac{2i}{n}\right)^2 - 1\right)^2\right), \tag{15}$$

...

Question 0.6. Let $f(\theta)$ be the function given by

$$f(\theta) = \frac{ab}{(a^2 + b^2) - (a^2 - b^2)\cos\theta} \qquad \theta \in [0, 2\pi] \tag{16}$$

with $a = 2$ and $b = 1$. Write a C/C++ computer program to apply the composite trapezoidal rule to evaluate the integral

$$I = \int_0^{2\pi} f(\theta) \mathrm{d}\theta \tag{17}$$

[1] https://www.wolframalpha.com/input?i=%5Cint_0%5E1+e%5E%7B-%5Cfrac%7Bx%5E2%7D%7B2%7D%7D

by dividing the interval $[0, 2\pi]$ into n sub-intervals $\{\theta_i, \theta_{i+1}\}_{i=0}^{n-1}$ with $\theta_i = 2\pi i/n$. For $n = 2, 4, 8, 16, 32$, print out the computed integrals and check the convergence rate (accuracy order) of the solution as n increases (Based on what you computed, make a guess on the exact value of the integral). Explain on what you observe.

解. $f(\theta)$ 存在初等原函数如下

$$\int f(\theta)\mathrm{d}\theta = \arctan\left(\frac{a}{b}\tan\frac{\theta}{2}\right) + C, \tag{18}$$

注意到原函数在 $\theta = \pi$ 处的间断点, 本题解析解为

$$I = \int_0^{\pi} f(\theta)\mathrm{d}\theta + \int_{\pi}^{2\pi} f(\theta)\mathrm{d}\theta = \frac{\pi}{2} + \frac{\pi}{2} = \pi. \tag{19}$$

使用梯形积分, 本题计算公式为

$$I_n = \frac{2\pi}{n}\left(\frac{1}{2}\left(\frac{a}{2b} + \frac{a}{2b}\right) + \sum_{i=0}^{n-1}\frac{ab}{(a^2+b^2) - (a^2-b^2)\cos\frac{2\pi i}{n}}\right), \tag{20}$$

Question 0.7. Find the quadrature points x_0, x_1 and the quadrature weights ω_0, ω_1 for a numerical quadrature of the form

$$\int_0^1 \frac{1}{\sqrt{x}} f(x)\mathrm{d}x \approx \omega_0 f(x_0) + \omega_1 f(x_1) \tag{21}$$

whose algebraic precision equals three.[2]

解. 首先构造区间为 $[0, 1]$, 权函数为 $\frac{1}{\sqrt{x}}$ 的二次正交多项式, 其零点为 Gauss 求积公式的节点. continue

Question 0.8. Let us consider evaluating the integral below

$$I = \int_0^1 e^{-t}\mathrm{d}t \tag{22}$$

with different composite methods at evenly spaced points $\{x_i = i/n\}_{i=0}^{n}$ for $n = 2, 4, 8, 16$ and 32. Print out the computed values and check the convergence rate (accuracy order) of the numerical integrals as n increases.

(a) apply the composite Simpson’ s rule;

(b) apply the composite two-node Gauss-Legendre quadrature;

(c) apply the composite three-node Gauss-Legendre quadrature.

解. 原积分存在解析解

$$I = -e^{-t}\Big|_0^1 = 1 - e^{-1}. \tag{23}$$

(a) 复合 Simpson 积分公式如下

$$\begin{aligned} S_n(f) &= \frac{h}{6}\sum_{k=1}^{n}[f(x_{k-1}) + 4f(x_{k-\frac{1}{2}}) + f(x_k)] \\ &= \frac{h}{6}\left[f(a) + 4\sum_{k=1}^{n} f(x_{k-\frac{1}{2}}) + 2\sum_{k=1}^{n-1} f(x_k) + f(b)\right], \end{aligned} \tag{24}$$

[2] [1]294 页例题 4.2

(b) $P_2(x) = \frac{1}{2}(3x^2 - 1)$.

(c) $P_3(x) = \frac{1}{2}(5x^3 - 3x)$.

Question 0.9. Apply the composite midpoint rule to compute the integral

$$I \equiv \int_0^1 \frac{4}{1+x^2} \mathrm{d}x = \pi \tag{25}$$

with

$$I_n^{(0)} \equiv \frac{1}{n} \sum_{i=0}^{n-1} \frac{4}{1+x_{i+1/2}^2} \tag{26}$$

and

$$x_{i+1/2} = \frac{1}{n}(i + \frac{1}{2}) \quad \text{for } i = 0, 1, \cdots, n-1. \tag{27}$$

Please first compute the numerical integral $I_n^{(0)}$ for each $n \in \{4, 8, 16, 32\}$. Compute other approximate integrals by the Richardson extrapolation technique (Romberg integration) for the composite midpoint rule, i.e.,

$$I_n^{(k+1)} = \frac{4^{k+1} I_n^{(k)} - I_{n/2}^{(k)}}{4^{k+1} - 1}. \tag{28}$$

Let

$$e_n^{(k)} = I - I_n^{(k)} \tag{29}$$

be the numerical error for each n and k. Please generate two tables as follows and study on the convergence rate (accuracy order) of the approximate integral $I_n^{(k)}$ as the number n of intervals increases for each fixed $k \in \{0, 1, 2, 3\}$.

表 3: Computed integrals by the composite midpoint rule

n	4	8	16	32
$I_n^{(0)}$				
$I_n^{(1)}$				
$I_n^{(2)}$				
$I_n^{(3)}$				

表 4: Numerical errors of the computed integrals by the composite midppoint rule

n	4	8	16	32
$e_n^{(0)}$				
$e_n^{(1)}$				
$e_n^{(2)}$				
$e_n^{(3)}$				

参考文献

[1] 陆金甫 关治. 数值分析基础. 3rd ed. 高等教育出版社, 2019.

附录