Problems of Chapter 6

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6.6.1-I Simpson's rule.

(a) Show that Simpson's rules on $[-1,1]$ can be obtained by

$$\int_{-1}^{1} y(t)\mathrm{d}t = \int_{-1}^{1} p_3(y;-1,0,0,1;t)\mathrm{d}t + E^S(y),$$

where $y \in C^4[-1,1]$ and $p_3(y;-1,0,0,1;t)$ is the interpolation polynomial of y that satisfies $p_3(-1)=y(-1)$, $p_3(0)=y(0)$, $p_3{\prime}(0)=y{\prime}(0)$, and $p_3(1)=y(1)$.

(b) Derive $E^S(y)$.

(c) Using (a), (b), and a change of variable, derive the composite Simpson's rules and prove the theorem on its error estimation.

解.

(a)

$$\begin{aligned}
&\int_{-1}^{1} P_3(y;-1,0,0,-1;t)\mathrm{d}t\\
=&\int_{-1}^{1}\left[y(-1)+y[-1,0](t+1)+y[-1,0,0]t(t+1)+y[-1,0,0,1](t+1)^2t\right]\mathrm{d}t\\
=&2y(-1)+2\left(y(0)-y(-1)\right)+\frac{2}{3}\left(y'(0)-y(0)+y(1)\right)+\frac{2}{3}\cdot\frac{1}{2}\left(y(1)-2y'(0)-y(-1)\right)\\
=&\frac{1}{3}\left(y(-1)+4y(0)+y(1)\right)=I^S(y).
\end{aligned}$$

(b)

$$E^S(y)=\int_{-1}^{1} y(t)\mathrm{d}t-\frac{1}{3}\left(y(-1)+4y(0)+y(1)\right).$$

(c)

$$\begin{aligned}
I_n^S(y)=&\int_{x_0}^{x_2} P_3(y;x_0,x_1,x_1,x_2;t)\mathrm{d}t+\int_{x_2}^{x_4} P_3(y;x_2,x_3,x_3,x_4)\mathrm{d}t+\cdots\\
&\int_{x_{n-2}}^{x_n} P_3(y;x_{n-2},x_{n-1},x_{n-1},x_n)\mathrm{d}t\\
\xlongequal{h=x_1-x_0=x_2-x_1}&\frac{h}{3}(y(x_0)+4y(x_1)+y(x_2))+\frac{h}{3}(y(x_2)+4y(x_3)+4y(x_4))+\cdots\\
&+\frac{h}{3}(y(x_{n-2}+4y(x_{n-1})+y(x_n)))\\
=&\frac{h}{3}(y(x_0)+4y(x_1)+2y(x_2)+4y(x_3)+\cdots+4y(x_{n-2})+y(x_n)).
\end{aligned}$$

这与 Def 6.19 中给出的公式相同。

$$
\begin{aligned}
E^S(y) &= \int_{-1}^{1} [y(t) - P_3(y; -1, 0, 0, 1; t)]\mathrm{d}t \xlongequal{Thm2.37} \int_{-1}^{1} \frac{f^{(4)}(\xi(t))}{24} t^2(t-1)(t+1)\mathrm{d}t \\
&= -\int_{-1}^{1} \frac{f^{(4)}(\xi(t))}{24} t^2(1-t)(t+1)\mathrm{d}t = -\frac{f^{(4)}(\xi)}{24} \int_{-1}^{1} t^2(1-t)(1+t)\mathrm{d}t \\
&= -\frac{f^{(4)}(\xi)}{24} \times \frac{4}{15} = -\frac{f^{(4)}(\xi)}{90} \\
E_n^S(y) &= \sum_{k=0}^{\frac{n}{2}-1} -\frac{f^{(4)}(\xi_k)}{90} \cdot h^5 = -\frac{f^{(4)}(\xi)}{90} \cdot h^5 \cdot \frac{n}{2} = -\frac{b-a}{180} h^4 f^{(4)}(\xi).
\end{aligned}
$$

□

6.6.1-II

Estimate the number of subintervals required to approximate $\int_0^1 e^{-x^2}\mathrm{d}x$ to six correct decimal places, i.e. the absolute error is less than 0.5×10^{-6},

(a) by the composite trapezoidal rule,

(b) by the composite Simpson's rule.

解.

$$
I = \int_0^1 e^{-x^2}\mathrm{d}x \approx 0.746824133
$$

本题求解代码如下：

```
#include<bits/stdc++.h>
using namespace std;
double f(double x) { return exp(-x*x); }
int main() {
    double I = 0.746824133;
    auto solveA = [&](){
        for(int N = 1; N <= 1000; ++N) {
            double h = 1.0 / N, tmp = 0.5*(f(0) + f(1));
            for(int i = 1; i < N; ++i) tmp += f(i*h); tmp /= N;
            if(fabs(tmp-I) < 5e-7) {
                cout << "Need " << N << " subintervals.->I_N^T = " << fixed << setprecision(9)
                     << tmp << ".\n";
                break;
            }
        }
    };
    auto solveB = [&](){
        for(int N = 1; N <= 1000; ++N) {
            double h = 1.0 / N, double tmp = f(0) + f(1);
            for(int i = 1; i < N; ++i) tmp += ((i&1)?4:2)*f(i*h); tmp/=N*3;
            if(fabs(tmp-I) < 5e-7) {
                cout << "Need " << N << " subintervals.->I_N^S = " << fixed << setprecision(9)
                     << tmp << ".\n";
                break;
            }
        }
    };
    solveA(); solveB();
}
```

输出结果为:

```
Need 351 subintervals.->I_N^T = 0.746823635.
Need 12 subintervals.->I_N^S = 0.746824526.
```

(a)

$$I_n^T(f) = h\left(\frac{1}{2}f(0) + f(h) + f(2h) + \cdots + f((n-1)h) + \frac{1}{2}f(1)\right)$$

$$I_{351}^T \approx 0.746823635, \quad E_{351}^T \approx 4.98 \times 10^{-7}.$$

所以至少需要 351 个子区间。

(b)

$$I_n^T(f) = \frac{h}{3}\left(f(0) + 4f(h) + 2f(2h) + \cdots + f(1)\right)$$

$$I_{12}^T \approx 0.746824526, \quad E_{12}^T \approx 4.13 \times 10^{-7}.$$

所以至少需要 12 个子区间。

□

6.6.1-III Gauss-Laguerre quadrature formula

(a) Construct a polynomial $\pi_2(t) = t^2 + at + b$ that is orthogonal to $\mathbb{P}_1$ with respect to the weght function $\rho(t) = e^{-t}$, i.e.

$$\forall p \in \mathbb{P}_1, \int_0^{+\infty} p(t)\pi_2(t)\rho(t)\mathrm{d}t = 0.$$

(hint : $\int_0^{+\infty} t^m e^{-t}\mathrm{d}t = m!$)

(b) Derive the two-point Gauss-Laguerre quadrature formula

$$\int_0^{+\infty} f(t)e^{-t}\mathrm{d}t = w_1 f(t_1) + w_2 f(t_2) + E_2(f)$$

and express $E_2(f)$ in terms of $f^{(4)}(\tau)$ for some $\tau > 0$.

(c) Apply the formula in (b) to approximate

$$I = \int_0^{+\infty} \frac{1}{1+t}e^{-t}\mathrm{d}t.$$

Use the remainder to estimate the error and compare your estimate with the true error. With the true error, identify the unknown quantity τ contained in $E_2(f)$.

(hint : use the exact value $I = 0.596347361\cdots$)

解.

(a)

$$\int_0^{+\infty} \pi_2(t)\rho(t)\mathrm{d}t = \int_0^{+\infty} (t^2 + at + b)e^{-t}\mathrm{d}t = 2 + a + b = 0$$

$$\int_0^{+\infty} \pi_2(t)\rho(t)t\mathrm{d}t = \int_0^{+\infty} (t^2 + at + b)te^{-t}\mathrm{d}t = 6 + 2a + b = 0$$

$$\Rightarrow a = -4, b = 2, \pi_2(t) = t^2 - 4t + 2.$$

(b)

$$\pi_2(t) = t^2 - 4t + 2 = 0 \Rightarrow t_1 = 2 - \sqrt{2}, t_2 = 2 + \sqrt{2}.$$

$$I(1) = I_2(1) \Rightarrow w_1 + w_2 = \int_0^{\infty} \rho(\tau)\mathrm{d}t = \int_0^{+\infty} e^{-t}\mathrm{d}t = 1.$$

$$I(t) = I_2(t) \Rightarrow w_1 t_1 + w_2 t_2 = \int_0^{+\infty} t\rho(t)\mathrm{d}t = \int_0^{+\infty} te^{-t}\mathrm{d}t = 1.$$

$$\Rightarrow w_1 = \frac{2+\sqrt{2}}{4}, w_2 = \frac{2-\sqrt{2}}{4}.$$

$$\int_0^{+\infty} f(t)e^{-t}\mathrm{d}t = \frac{2+\sqrt{2}}{4} f(2-\sqrt{2}) + \frac{2-\sqrt{2}}{4} f(2+\sqrt{2}) + E_2(f).$$

$$E_2(f) = \frac{f^{(4)}(\tau)}{24}\int_0^{+\infty} e^{-t}(t^2-4t+2)^2\mathrm{d}t = \frac{f^{(4)}(\tau)}{6}.$$

(c)

$$I_2(f) = \frac{2+\sqrt{2}}{4}\cdot\frac{1}{1+2-\sqrt{2}} + \frac{2-\sqrt{2}}{4}\cdot\frac{1}{1+2+\sqrt{2}} = \frac{4}{7} \approx 0.571428571.$$

$$E_2(f) = I(f) - I_2(f) \approx 0.024918790.$$

$$f^{(4)}(t) = \left(\frac{1}{1+t}\right)^{(4)} = \frac{24}{(1+t)^5}$$

$$\frac{24}{6(1+\tau)^5} = E_2(f) \Rightarrow \tau \approx 1.76126.$$

□

6.6.1-IV Remainder of Gauss formulas

Consider the Hermite interpolation problem: find $p \in \mathbb{P}_{2n-1}$ such that

$$\forall m = 1, 2, \cdots, n, p(x_m) = f_m, p'(x_m) = f'_m. \qquad (6.44)$$

There are *elementary Hermite interpolation polynomials* h_m, q_m such that the solution of (6.44) can be expressed in the form

$$p(t) = \sum_{m=1}^{n}[h_m(t)f_m + q_m(t)f'_m],$$

analogous to the Lagrange interpolation formula.

(a) Seek h_m and q_m in the form

$$h_m(t) = (a_m + b_m t)\ell_m^2(t), q_m(t) = (c_m + d_m t)\ell_m^2(t)$$

where ℓ_m is the elementary Lagrange polynomial in (2.9). Determine the constants a_m, b_m, c_m, d_m.

(b) Obtain the quadrature rule

$$I_n(f) = \sum_{k=1}^{n}[w_k f(x_k) + \mu_k f'(x_k)]$$

that satisfies $E_n(p) = 0$ for all $p \in \mathbb{P}_{2n-1}$.

(c) What conditions on the node polynomial or on the nodes x_k must be imposed so that $\mu_k = 0$ for each $k = 1, 2, \cdots, n$?

解.

(a)

$$p(x_m) = \sum_{k=1}^{n}\left[h_k(x_m)f_k + q_k(x_m)f'_k\right] = \sum_{k=1}^{n}\left[(a_k + b_k x_m)f_k + (c_k + d_k x_m)f'_k\right]\ell_k^2(x_m)$$

$$= (a_m + b_m x_m)f_m + (c_m + d_m x_m)f'_m = f_m$$

$$p'(x_m) = \sum_{k=1} n\left[h'_k(x_m)f_k + q'_k(x_m)f'_k\right]$$

$$= \sum_{k=1}^{n}\left[(b_k f_k + d_k f'_k)\ell_k(x_m) + [(a_k + b_k x_m)f_k + (c_k + d_k x_m)f'_k]2\ell'_k(x_m)\right]\ell_k(x_m)$$

$$= (b_m f_m + d_m f'_m) + 2\left[(a_m + b_m x_m)f_m + (c_m + d_m x_m)f'_m\right]\cdot\sum_{i\neq m}\frac{1}{x_m - x_i} = f'_m$$

$$\Rightarrow \begin{cases} a_m + x_m b_m = 1 \\ c_m + x_m d_m = 0 \\ 2(a_m + x_m b_m)\ell_m'(x_m) + b_m = 0 \\ 2(c_m + x_m d_m)\ell_m'(x_m) + d_m = 1 \end{cases} \Rightarrow \begin{cases} a_m = 1 + 2x_m \ell_m'(x_m) \\ b_m = -2\ell_m'(x_m) \\ c_m = -x_m \\ d_m = 1 \end{cases} \quad (l_m'(x_m) = \sum_{i \neq m} \frac{1}{x_m - x_i})$$

(b) 令 $I_n(f) = \int_a^b p(t)\mathrm{d}t = \sum_{k=1}^n \left[w_k f(x_k) + \mu_k f'(x_k)\right]$.

其中，$w_k = \int_a^b h_k(t)\mathrm{d}t = \int_a^b \left[1 + 2(x_k - t)\ell_k'(x_k)\right]\ell_k^2(t)\mathrm{d}t$，$\mu_k = \int_a^b q_k(t)\mathrm{d}t = \int_a^b (t - x_k)\ell_k^2(t)\mathrm{d}t$。

因为 $p(t)$ 是对 f 的 $2n-1$ 次 Hermite 插值，所以对 $p \in \mathbb{P}_{2n-1}, p(t) \equiv f$.

即 $\forall p \in \mathbb{P}_{2n-1}, E_n(p) = 0$.

(c) 需满足：

$$\forall k, \mu_k = \int_a^b (t - x_k)\ell_k^2(t)\mathrm{d}t = \int_a^b \frac{V_n^2(t)}{t - x_k}\mathrm{d}t = 0.$$

□

6.6.1-V

Prove Lemma 6.43.

> In approxmating the second derivative of $u \in C^4(\mathbb{R})$, the formula
> $$D^2u(\bar{x}) = \frac{u(\bar{x} - h) - 2u(\bar{x}) + u(\bar{x} + h)}{h^2}$$
> is second-order accurate. Furthermore, if the input function values $u(\bar{x} - h)$, $u(\bar{x})$, and $u(\bar{x} + h)$ are perturbed with random errors $\epsilon \in [-E, E]$, then there exists $\xi \in [\bar{x} - h, \bar{x} + h]$ such that
> $$|u''(\bar{x}) - D^2u(\bar{x})| \leq \frac{h^2}{12}|u^{(4)}(\xi)| + \frac{4E}{h^2}.$$

How do you choose h to minimize the error bound in (6.43)? Design a fourth-order accurate formula based on a symmetric stencil, derive its error bound, and minimize the error bound. What do you observe in comparing the second-order case and the fourth-order case?

证明.

1.
$$\begin{aligned} D^2u(\bar{x}) &= \frac{u(\bar{x} - h) - 2u(\bar{x}) + u(\bar{x} + h)}{h^2} \\ &= \frac{1}{h^2}[u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) - \frac{h^3}{6}u'''(\bar{x}) + \frac{h^4}{24}u^{(4)}(\bar{x}) - \frac{h^5}{120}u^{(5)}(\bar{x}) - 2u(\bar{x}) \\ &\quad + u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \frac{h^3}{6}u'''(\bar{x}) + \frac{h^4}{24}u^{(4)}(\bar{x}) + \frac{h^5}{120}u^{(5)}(\bar{x}) + O(h^6)] \\ &= u''(\bar{x}) + \frac{h^2}{12}u^{(4)}(\bar{x}) + O(h^{(4)}). \end{aligned}$$

所以 $|u''(\bar{x}) - D^2u(\bar{x})| = \frac{h^2}{12}|u^{(4)}(\xi)|, \quad \xi \in (\bar{x} - h, \bar{x} + h)$。

当 u 的计算存在误差 $\varepsilon \in [-E, E]$ 时，

$$|u''(\bar{x}) - D^2\tilde{u}(\bar{x})| \leq |u''(\bar{x}) - D^2u(\bar{x})| + |D^2u(\bar{x}) - D^2\tilde{u}(\bar{x})| \leq \frac{h^2}{12}|u^{(4)}(\xi)| + \frac{4E}{h^2}.$$

2. 取 $h = \left(\frac{|u^{(4)}(\bar{x})|}{12} \cdot 4E\right)^{\frac{1}{4}} = \left(\frac{E|u^{(4)}(\bar{x})|}{3}\right)^{\frac{1}{4}}$，误差上界为 $2\left(\frac{E \cdot \max_{x \in [\bar{x} - h, \bar{x} + h]} |u^{(4)}(x)|}{3}\right)^{\frac{1}{2}}$。

3. 设

$$
\begin{aligned}
D_2^2u(\bar{x}) &= \frac{Au(\bar{x}-2h)+Bu(\bar{x}-h)+Cu(\bar{x})+Bu(\bar{x}+h)+Au(\bar{x}+2h)}{h^2} \\
&= \frac{1}{h^2}\left[(2A+2B+C)u(\bar{x})+(4A+B)h^2u''(\bar{x})+\frac{1}{12}(16A+B)h^4u^{(4)}(\bar{x})+\frac{1}{360}(64A+B)h^6u^{(6)}(\bar{x})+O(h^8)\right]
\end{aligned}
$$

所以 $\begin{cases} 2A+2B+C=0 \\ 4A+B=0 \\ 16A+B=0 \end{cases} \Rightarrow \begin{cases} A=-\frac{1}{12} \\ B=\frac{4}{3} \\ C=-\frac{5}{2} \end{cases}$

即 $D_2^2u(\bar{x}) = \dfrac{-u(\bar{x}-2h)+16u(\bar{x}-h)-30u(\bar{x})+16u(\bar{x}+h)-u(\bar{x}+2h)}{12h^2}$

$D_2^2u(\bar{x}) = u''(\bar{x})+\dfrac{h^4}{360}(64A+B)u^{(6)}(\bar{x}) = u''(\bar{x})-\dfrac{h^4}{90}u^{(6)}(\bar{x})+O(h^{(6)})$.

当 u 的计算存在误差 $\varepsilon\in[-E,E]$ 时，

$$
|u''(\bar{x})-D_2^2\tilde{u}(\bar{x})| \le \frac{h^4}{90}|u^{(6)}(\xi)|+\frac{16E}{3h^2}. \quad \xi\in(x-2h,x+2h).
$$

取 $h=\left(\dfrac{|u^{(6)}(\bar{x})|}{90}\cdot\dfrac{16E}{3}\cdot\dfrac{1}{2}\right)^{\frac{1}{6}} = \left(\dfrac{4E|u^{(6)}(\bar{x})|}{135}\right)^{\frac{1}{6}}$，误差上界为 $3\left(\dfrac{640E^2}{|u^{(6)}(\bar{x})|}\right)^{\frac{1}{3}}$。

4. (a) 四阶精度的误差上界只在二阶精度的 $O(E^{\frac{1}{2}})$ 基础上提升到 $O(E^{\frac{2}{3}})$；

   (b) 二阶精度公式的误差上界和 u 的高阶导数正相关，但四阶精度公式误差上界和 u 的高阶导数负相关。

□

参考文献

[1] 张庆海. “Notes on Numerical Analysis and Numerical Methods for Differential Equations”. In: (2023).