

## Chapter 9

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**Problem 9.1.** Simpson's rule.

(a) Show that on  $[-1, 1]$  Simpson's rule can be obtained as follows

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

where  $y \in C^4[-1, 1]$  and  $p_3(y; -1, 0, 0, 1; t)$  is the interpolation polynomial of  $y$  with interpolation conditions  $p_3(-1) = y(-1)$ ,  $p_3(0) = y(0)$ ,  $p_3'(0) = y'(0)$ , 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 rule and prove the theorem on its error estimation.

**Solution.**

(a) By interpolating, we can get  $p_3(y; -1, 0, 0, 1; t) = y(-1) + (y(0) - y(-1))(x+1) + (y'(0) - y(0) + y(-1))x(x+1) + (\frac{y(1)-y(-1)-2y'(0)}{2})x^2(x+1)$ . Integrate  $p_3$  get  $\int_{-1}^1 p_3(y; -1, 0, 0, 1; t)dt = \frac{1}{3}(f(-1) + 4f(0) + f(1))$ .

(b) Since  $y(x) - p_3(y; x) = \frac{y^{(4)}(x)}{4!}(x+1)x^2(x-1)$ , therefore

$$\begin{aligned} E^S(y) &= \int_{-1}^1 y(t) - p_3(y; -1, 0, 0, 1; t)dt \\ &= \int_{-1}^1 \frac{y^{(4)}(t)}{4!}(t+1)t^2(t-1)dt \\ &= -\frac{1}{90}f^{(4)}(\zeta). \end{aligned}$$

(c)

$$\begin{aligned} E^S(f) &= \int_a^b f(t)dt - \frac{b-a}{6} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] \\ &= \int_a^b f(t)dt - \int_a^b p_3(f; a, \frac{a+b}{2}, \frac{a+b}{2}, b; t)dt \\ &= \int_a^b \frac{f^{(4)}(t)}{4!}(t-a)(t-\frac{a+b}{2})^2(t-b)dt \\ &= -\frac{(b-a)^5}{2880}f^{(4)}(\zeta). \end{aligned}$$

**Problem 9.2.** Estimate the number of subintervals required to approximate  $\int_0^1 e^{-x^2} dx$  to 6 correct decimal places, i.e. the absolute error is no greater than  $0.5 \times 10^{-6}$ ,

(a) by the composite trapezoidal rule.

(b) by the composite Simpson's rule.

**Solution.**

(a) Let  $f(x) = e^{-x^2}$ , we have  $|f^{(2)}(x)| = |4x^2e^{-x^2} - 2e^{-x^2}| < 2$ . So by the composite trapezoidal rule,  $|E_n^T(f)| < 0.5 \times 10^{-6} \iff \frac{1}{6}h^2 < \frac{1}{2} \times 10^{-6}$ . Therefore, the number of subintervals is about  $\frac{1}{h} = 578$ .

(b) We also have  $|f^{(4)}(x)| < 30$ ,  $|E_n^S(f)| < 0.5 \times 10^{-6} \iff \frac{1}{6}h^4 < \frac{1}{2} \times 10^{-6}$ . Therefore, the number of subintervals is about 25.

**Problem 9.3.** Gauss-Larguerre quadrature formula.

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

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

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

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

$$\int_0^{+\infty} f(t)e^{-t}dt = w_1f(t_1) + w_2f(t_2) + E_2(f)$$

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

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

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

Use the remainder to estimate the error and compare your estimate with the true error. With the true error, identify the unknown quantity  $\tau$  contained in  $E_2(f)$ . (hint; use the exact value  $I = 0.596347361 \dots$ )

**Solution.**

(a) Since  $\pi_2(t)$  is orthogonal to  $\mathbb{P}_1$  indicate that  $\langle \pi_2, 1 \rangle = \langle \pi_2, t \rangle = 0$ ,

$$\begin{aligned} \langle \pi_2, 1 \rangle &= \int_0^{\infty} e^{-t}(t^2 + at + b)dt \\ &= 2! + 1!a + 0!b = 2 + a + b = 0 \\ \langle \pi_2, t \rangle &= \int_0^{\infty} e^{-t}(t^3 + at^2 + b)t dt \\ &= 3! + 2!a + 1!b = 6 + 2a + b = 0. \end{aligned}$$

Solve this get  $a = -4, b = 2$ .

(b) By (a) get  $t_1 = 2 + \sqrt{2}, t_2 = 2 - \sqrt{2}$ . And choose  $f_1(t) = 1, f_2(t) = t$  respectively give

$$\begin{aligned} w_1 \cdot 1 + w_2 \cdot 1 &= \int_0^{\infty} 1e^{-t}dt = 1 \\ w_1 t_1 + w_2 t_2 &= \int_0^{\infty} te^{-t}dt = 1. \end{aligned}$$

Solves this equations get  $w_1 = \frac{2-\sqrt{2}}{4}, w_2 = \frac{2+\sqrt{2}}{4}$ .  $E_2(f) = \frac{f^{(4)}(\tau)}{4!} \int_0^{+\infty} e^{-t}(t^2-4t+2)^2 dt = \frac{f^{(4)}(\tau)}{4!} \int_0^{+\infty} e^{-t}(t^4-8t^3+20t^2-16t+4)dt = \frac{f^{(4)}(\tau)}{4!}(4!-8 \times 3!+20 \times 2!-16 \times 1!+4 \times 0!) = \frac{f^{(4)}(\tau)}{6}$ .

- (c) The remainder  $E_2(\frac{1}{1+t}) = \frac{4}{(1+t)^5}$ , the true error  $e = I - w_1 f(t_1) - w_2 f(t_2) = 0.0249187896 = \frac{4}{(1+\tau)^5} \implies \tau = 1.7612556$ .

## 9.1 Program

Write a **C++** function to perform discrete least square via QR factorization. Your algorithm should take as input the maximum degree of the fitting polynomial, three or more data pairs  $(x_i, y_i)$ , and output coefficients of the fitted polynomial.

Run your subroutine on the following data.

x	0.0	0.5	1.0	1.5	2.0	2.5	3.0
y	2.9	2.7	4.8	5.3	7.1	7.6	7.7
x	3.5	4.0	4.5	5.0	5.5	6.0	6.5
y	7.6	9.4	9.0	9.6	10.0	10.2	9.7
x	7.0	7.5	8.0	8.5	9.0	9.5	10.0
y	8.3	8.4	9.0	8.3	6.6	6.7	4.1

In the note, the condition number a matrix  $A$  is defined as

$$\text{cond}_A(\mathbf{x}) = \|A\| \|A^{-1}\|.$$

Report the condition number based on the 2-norm of matrix  $G$  in the normal equation approach (reuse results of your previous homework!) and that of the matrix  $R_1$  in the QR-factorization approach, verifying that the former is much larger than the latter.

*make run* will output the polynomial on terminal and use **matlab** calculate the condition number. Matlab will output  $A, A^{-1}, \|A\|_2, \|A^{-1}\|_2, \|A\|_2 \|A^{-1}\|_2$  respectively. The condition numbers are  $1.8981 \times 10^4, 137.7715$ , which shows that former is much larger.