A Numerical Analysis Problem Book

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Preface

This is the preface. It is an unnumbered chapter. The `markboth` TeX field at the beginning of this paragraph sets the correct page heading for the Preface portion of the document. The preface does not appear in the table of contents.

Introduction

The introduction is entered using the usual chapter tag. Since the introduction chapter appears before the `mainmatter` TeX field, it is an unnumbered chapter. The primary difference between the preface and the introduction in this shell document is that the introduction will appear in the table of contents and the page headings for the introduction are automatically handled without the need for the `markboth` TeX field. You may use either or both methods to create chapters at the beginning of your document. You may also delete these preliminary chapters.

Chapter 1

Errors and FPA

Problem 1 (Gautschi, Ch.1, 35, pag.49) *Consider the algebraic equation*

$$x^n + ax - 1 = 0, \quad a > 0, \; n \geq 2.$$

(a) Show that the equation has exactly one positive root $\xi(a)$.

(b) Obtain a formula for $(cond\xi)(a)$.

(c) Obtain (good) upper and lower bounds for $(cond\xi)(a)$.

Solution. (a) $f'(x) = nx^{n-1} + a > 0$, for $x > 0$

$$f(0) = -1 < 0$$

$$f(1) = 1 + a - 1 = a > 0$$

$$f(x) > 0, \; \forall \; x > 1$$

f strictly increasing $\Rightarrow$ uniqueness of root in $(0, \infty)$.

(b) $(cond\xi)(a) = \left| \frac{a\frac{d\xi}{da}}{\xi} \right|$

ξ root $\Rightarrow \xi^n + a\xi - 1 = 0 \Big| \frac{d}{da}$

$$n\xi^{n-1}\frac{d\xi}{da} + \xi + a\frac{d\xi}{da} = 0$$

$$\frac{d\xi}{da}(n\xi^{n-1} + a) = -\xi$$

$$\frac{d\xi}{da} = \frac{-\xi}{n\xi^{n-1} + a}$$

$$(cond\xi)(a) = \left| \frac{a\dfrac{\xi}{n\xi^{n-1}+a}}{\xi} \right| = \frac{a}{n\xi^{n-1}+a}$$

(c) $0 < \xi < 1 \Rightarrow \dfrac{a}{a+n} < (cond\xi)(a) < 1$ ■

Problem 2 (Gautschi, Ch.1, 28, pag.47) *Let $f : \mathbb{R}^2 \to \mathbb{R}$ given by $y = x_1 + x_2$. Define $(condf)(x) = (cond_1 f)(x) + (cond_2 f)(x)$ where $cond_i f$ is the condition number of f considered a function of x_i only $(i = 1, 2)$.*

(a) Derive a formula for $k(x_1, x_2) = (condf)(x)$.

(b) Show that $k(x_1, x_2)$ as a function of x_1, x_2 is symmetric with respect to bisectors b_1 and b_2.

(c) Determine the lines (or domains) in $\mathbb{R}^2$ on which $k(x_1, x_2) = c$, $c \geq 1$ a constant.

(Simplify the analysis by using symmetry, cf. part (b)).

Solution. (a) $(cond_1 f)(x) = \left| \dfrac{x_1 \dfrac{\partial f}{\partial x_1}}{x_1 + x_2} \right| + \left| \dfrac{x_2 \dfrac{\partial f}{\partial x_2}}{x_1 + x_2} \right| = \dfrac{|x_1| + |x_2|}{|x_1 + x_2|} = k(x_1, x_2)$

(b) $k(x_1, x_2) = k(x_1, x_2)$, $k(-x_1, x_2) = k(x_1, x_2)$. ■

Chapter 2

Approximation and Interpolation

Problem 3 (Gautschi, Ch.2, 33, pag.133) *(a) Let $L_n(f;x)$ be the interpolation polynomial of degree $\le n$ interpolating $f(x) = e^x$ at the points $x_i = i/n$, $i = 0, 1, 2, \ldots, n$. Derive an upper bound for*

$$\max_{0\le x\le 1} |e^x - (L_n f)(x)| = \max_{0\le x\le 1} |(R_n f)(x)|$$

and determine the smallest n guaranteeing an error less than 10^{-6} on $[0, 1]$.

Hint. *First show that for any integer i with $0 \le i \le n$ one has*

$$\max_{0\le x\le 1} \left|\left(x - \frac{i}{n}\right)\left(x - \frac{n-i}{n}\right)\right| \le \frac{1}{4}.$$

(b) Solve the analogous problem for the n-th degree Taylor polynomial

$$(T_n f)(x) = 1 + x + \frac{x^2}{2!} + \cdots + \frac{x^n}{n!},$$

and compare the result with the one in (a).

Solution. $f(x) = e^x$, $x_i = i/n$, $i = \overline{0, n}$

$$(R_n f)(x) = \frac{e^\xi}{(n+1)!} \prod_{i=0}^{n} \left(x - \frac{i}{n}\right)$$

$$|(R_n f)(x)| \le \frac{e}{(n+1)!} \prod_{i=0}^{n} \left| x - \frac{i}{n} \right|$$

$$\left| \left(x - \frac{i}{n} \right) \left(x - \frac{n-i}{n} \right) \right| \le \frac{1}{4}$$

n odd $n = 2k+1$, $n+1 = 2(k+1)$

$$\left| \prod_{i=0}^{n} \left(x - \frac{i}{n} \right) \right| = \prod_{i=1}^{k+1} \left| \left(x - \frac{i}{n} \right) \left(x - \frac{n-i}{n} \right) \right| \le \frac{1}{4^{\frac{n+1}{2}}} = \frac{1}{2^{n+1}}$$

n even, $n+1 = 2k+1$

$$\left| x - \frac{k}{2k} \right| = \left| x - \frac{1}{2} \right| \le \frac{1}{2}$$

$$\left| \prod_{i=0}^{n} \left(x - \frac{i}{n} \right) \right| \le \frac{1}{2} \prod \left| \left(x - \frac{i}{n} \right) \left(x - \frac{n-i}{n} \right) \right| \le \frac{1}{2} \cdot \frac{1}{4^{\frac{n}{2}}} = \frac{1}{2^{n+1}}$$

$$2^n (n+1)! > \frac{10^6}{e}$$

$$|(R_n f)(x)| \le \frac{e}{2^{n+1}(n+1)!}$$

$$\frac{e}{2^n (n+1)!} < 10^{-6}$$

$$n = 7$$

(b) $(R_n f)(x) = \dfrac{x^{n+1}}{(n+1)!} e^{\xi}$

$$|(R_n f)(x)| \le \frac{e}{(n+1)!}$$

$$\frac{e}{(n+1)!} < 10^{-6}$$

$$n = 10$$

■

Problem 4 *(Gautschi, Ch.2, P.5, pag.126)*

Taylor expansion yields the simple approximation $e^x \approx 1 + x$, $0 \le x \le 1$. Suppose you want to improve this by seeking an approximation of the form $e^x \approx 1 + cx$, $0 \le x \le 1$, for some suitable c.

(a) How must c be chosen if the approximation is to be optimal in the (continuously, equally weighted) least squares sense?

(b) Sketch the error curves $e_1(x) = e^x - (1+x)$ and $e_2(x) = e^x - (1+cx)$ with c as obtained in (a) and determine $\max_{0\le x\le 1} |e_1(x)|$ and $\max_{0\le x\le 1} |e_2(x)|$.

(c) Solve an analogous problem (and provide error curves) with three instead of two terms in the modified Taylor expansion:

$$e^x \approx 1 + c_1 x + c_2 x^2.$$

Solution.

$$E^2 = \int_0^1 (e^x - 1 - cx)^2 dx \to \min \text{ (with respect to } c\text{)}$$

$$\frac{\partial E^2}{\partial c} = 2\int_0^1 (e^x - 1 - cx)(-x)dx = -1 + \frac{2}{3}c = 0$$

$$c = \frac{3}{2}$$

$$\varphi(x) = 1 - \frac{3}{2}x$$

$$e_1(x) = e^x - 1 - x$$

$$e_2(x) = e^x - 1 - \frac{3}{2}x$$

$$\max_{x\in[0,1]} |e_1| = e - 2 \approx 0.71 \; \max_{x\in[0,1]} |e_2| = e - \frac{5}{2} \approx 0.218$$

(b) $E^2 = \int_0^1 (e^x - 1 - c_1 x - c_2 x)^2 dx \to \min$

$$\begin{cases} \dfrac{\partial E^2}{\partial c_1} = -1 + \dfrac{2}{3}c_1 + \dfrac{1}{2}c_2 = 0 \\[2ex] \dfrac{\partial E_2}{\partial c_2} = \dfrac{14}{3} - 2e + \dfrac{1}{2}c_1 + \dfrac{2}{5}c_2 = 0 \end{cases}$$

$$c_1 = 164 - 60e, \quad c_2 = -\frac{650}{3} + 80e$$

$$\max_{x\in[0,1]} |e_1| = e - \frac{5}{2} \approx 0.218281828$$

$$\max_{x\in[0,1]} |e_2| = -19e + \frac{155}{3} \approx 0.1931194$$

■

Problem 5 (classical) *Given $f \in C[a,b]$, find $\widehat{s}_1(f;\cdot) \in S_1^0(\Delta)$ such that*

$$\int_a^b [f(x) - \widehat{s}_1(f;x)]^2 dx \to \min$$

using the base of first degree B-splines.

Solution. Writing

$$\widehat{s}_1(f;x) = \sum_{i=1}^{n} \widehat{c}_i B_i(x) \tag{1}$$

we know from the general theory that the coefficients $\widehat{c}_i$ must satisfy the normal equations

$$\sum_{j=1}^{n} \left[\int_a^b B_i(x) B_j(x) dx \right] c_j = \int_a^b B_i(x) f(x) dx, \quad i = \overline{1,n} \tag{2}$$

Now the fact that B_i is nonzero only on (x_{i-1}, x_{i+1}) implies that

$$\int_a^b B_i(x) B_j(x) dx = 0 \text{ if } |i-j| > 1;$$

that is the system (2) is tridiagonal. (Note that, we make the convention $\Delta x_0 = 0$ and $\Delta x_n = 0$). Its matrix is

$$\begin{bmatrix} \frac{1}{3}\Delta x_1 & \frac{1}{6}\Delta x_1 & & & 0 \\ \frac{1}{6}\Delta x_1 & \frac{1}{3}(\Delta x_1 + \Delta x_2) & \frac{1}{6}\Delta x_2 & \dots & \\ & \frac{1}{6}\Delta x_2 & & & \\ & & \ddots & \ddots & \frac{1}{6}\Delta x_{n-1} \\ 0 & & & \frac{1}{6}\Delta x_{n-1} & \frac{1}{3}\Delta x_{n-1} \end{bmatrix}$$

The matrix is symmetric and positive definite, but it is also diagonally dominant, each diagonal element exceeding the sum of the (positive) off-diagonal elements in the same row by a factor of 2. ■

Problem 6 (Gautschi, Ch.2, 40, pag.134) *(a) For quadratic interpolation equally spaced points x_0, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, derive an upper bound $\|R_2 f\|_\infty$ involving $\|f'''\|_\infty$ and h.*

(b) Compare the bound obtained in (a) with the analogous one for interpolation at three Chebyshev points in $[x_0, x_2]$.

Solution. (a) $(R_2f)(x) = \dfrac{(x-x_0)(x-x_0-h)(x-x_0-2h)}{3!}f'''(\xi)$

$$\|R_2f\| \le \frac{1}{3!}\|u\|_\infty \|f'''\|_\infty$$

$$u(x) = (x-x_0)(x-x_0-h)(x-x_0-2h)$$

$$u_{max} = \frac{2h^3}{3\sqrt{3}}$$

$$\|R_2f\| \le \frac{1}{6}\cdot\frac{2h^3}{3\sqrt{3}}\|f'''\|_\infty = \frac{h^3}{9\sqrt{3}}\|f'''\|_\infty$$

(b) $\|R_mf\|_\infty \le \dfrac{(b-a)^{m+1}}{(m+1)!2^{2m+1}}\|f^{(n+1)}\|_\infty \; m=2$

$$\|R_2f\|_\infty \le \frac{(2h^3)^3}{3!\cdot 2^5}\|f'''\|_\infty = \frac{h^3}{24}\|f'''\|_\infty$$

■

Problem 7 (Gautschi, Ch.2, 41, pag.134) *(a) Suppose the function $f(x) = \ln(2+x)$, $x \in [-1,1]$ is interpolated by a polynomial L_nf at the Cebyshev points $x_k = \cos\left(\frac{2k+1}{2n+2}\pi\right)$, $k = \overline{0,n}$. Derive a bound for the maximum error, $\|R_nf\|_\infty$.*

(b) Compare the result of (a) with a bound for $\|R_n^Tf\|_\infty$ the remainder of Taylor interpolation polynomial of f.

Solution. $f^{(n)}(x) = \dfrac{(-1)^{n-1}(n-1)!}{(x+2)^n}$

$$\|f^{(n+1)}\|_\infty = n!$$

$$\|R_nf\|_\infty \le \frac{1}{(m+1)!2^m}\|f^{(n+1)}\|_\infty = \frac{1}{(n+1)!2^n}n! = \frac{1}{2^n(n+1)}$$

(b) $(R_n^Tf)(x) = \dfrac{x^{n+1}}{(n+1)!}f^{(n+1)}(\xi)$

$$\|R_n^Tf\|_\infty \le \frac{1}{(n+1)!}n! = \frac{1}{n+1}$$

■

Problem 8 (Gautschi, Ch.2, p.42, pag.135) *Consider* $f(t) = \arccos t$, $t \in [-1, 1]$. *Obtain the least squares approximation* $\widehat{\varphi} \in P_n$ *of* f *relative to the weight function* $w(t) = (1-t^2)^{-\frac{1}{2}} = \frac{1}{sqrt1-t^2}$ *that is, find the solution* $\varphi = \widehat{\varphi}$ *of*

$$minimize \left\{ \int_{-1}^{1} [f(t) - \varphi(t)]^2 \frac{dt}{\sqrt{1-t^2}} : \ \varphi \in P_n \right\}.$$

Express φ *in terms of Cebyshev polynomials* $\pi_j(t) = T_j(t)$.

Solution. $\widehat{\varphi}(t) = \dfrac{c_0}{2} + c_1 T_1(x) + \cdots + c_n T_n(x)$

$$c_k = \frac{(f, T_k)}{(T_k, T_k)} = \frac{2}{\pi}(f, T_k) = \frac{2}{\pi}\int_{-1}^{1} \frac{\arccos t}{\sqrt{1-t^2}} \cos(k \arccos t) dt$$

$$= \frac{2}{\pi}\int_0^{\pi} u \cos ku du = \frac{2}{\pi}\left[\frac{u \sin ku}{k}\Big|_0^{\pi} - \frac{1}{k}\int_0^{\pi} \sin ku du \right]$$

$$= \frac{2}{\pi}\left[\frac{1}{k}\frac{\cos ku}{k}\Big|_0^{\pi} \right] = -\frac{2}{\pi k^2}[(-1)^k - 1]$$

k even $c_k = 0$

k odd $c_k = -\dfrac{2}{\pi k^3}(-2) = \dfrac{4}{\pi k^2}$ ■

Problem 9 *(Gautschi, Ch.2, 43, pag.135)*

Compute $T_n'(0)$, *where* T_n *is the Cebyshev polynomial of degree* n.

Solution. $T_n'(x) = [\cos u \arccos x]' = \dfrac{-\sin n \arccos x}{-\sqrt{1-x^2}} = Q_{n-1}(x)$

$$T_n'(0) = Q_n(0) = \sin n \arccos 0 = \sin n$$

■

Problem 10 *(Gautschi, Ch.2, 7, pag.126)*

Determine the least square approximation

$$\varphi(t) = \frac{c_1}{1+t} + \frac{c_2}{(1+t)^2}, \quad t \in [0, 1]$$

to the exponential function $f(t) = e^{-t}$, *assuming* $d\lambda(t) = dt$ *on* $[0, 1]$. *Determine the condition number* $cond_{\infty} A = \|A\|_{\infty} \|A^{-1}\|_{\infty}$ *of the coefficient* *matrix A of the normal equations. Calculate the error $f(t) - \varphi(t)$ at $t = 0$, $t = 1/2$, and $t = 1$.*

(Point of information: The integral

$$\int_1^\infty t^{-m} e^{-xt} dt = E_m(x) = E_i(m, x)$$

is known as the "mth exponential integral".)

Solution. Normal equations

$$\varphi_0(t) = \frac{1}{1+t}$$

$$\varphi_1(t) = \frac{1}{(1+t)^3}$$

$$(\varphi_0, \varphi_0)c_0 + (\varphi_0, \varphi_1)c_1 = (f, \varphi_0)$$

$$(\varphi_0, \varphi_1)c_0 + (\varphi_1, \varphi_1)c_1 = (f, \varphi_1)$$

$$(\varphi_0, \varphi_0) = \int_0^1 \frac{dt}{(1+t)^2} = -\frac{1}{1+t}\Big|_0^1 = \frac{1}{2}$$

$$(\varphi_0, \varphi_1) = \int_0^1 \frac{dt}{(1+t)^3} = \frac{3}{8}$$

$$(\varphi_1, \varphi_1) = \int_0^1 \frac{dt}{(1+t)^4} = \frac{7}{24}$$

$$b_1 = \int_0^1 \frac{e^{-t}}{1+t} dt = e[E_i(1,1) - E_i(1,2)]$$

$$B_2 = \int_0^1 \frac{e^{-t}}{(1+t)^2} dt = e[E_i(1,2) - E_i(1,1)] - \frac{1}{2e}$$

solutions

$$c_0 = -128 E_i(1,2)e + 128 E_i(1,1)e + \frac{36}{e} - 72$$

$$c_1 = 168 E_i(1,2)e - 168 E_i(1,1)e - \frac{48}{e} + 96$$

$$\varphi(t) = \frac{c_0}{1+t} + \frac{c_1}{(1+t)^3}$$

$$A = \begin{bmatrix} \frac{1}{2} & \frac{3}{8} \\ \frac{3}{8} & \frac{7}{24} \end{bmatrix} \qquad A^{-1} = \begin{bmatrix} 56 & -72 \\ -72 & 96 \end{bmatrix}$$

$$cond_{\infty}A = \|A\|_{\infty}\|A^{-1}\|_{\infty} = \frac{7}{8}\cdot 168 = 147$$

Errors
$t = 0$

$$-23 - 40E_i(1,2)e + 40E_i(1,1)e + \frac{12}{e} \approx -0.048566996$$

$t = 1/2$

$$e^{-\frac{1}{2}} + \frac{32}{3}E_i(1,2)e - \frac{32}{3}E_i(1,1)e - \frac{8}{3e} + \frac{16}{3} \approx 0.015684228$$

$t = 1$

$$-\frac{5}{e} + 22E_i(1,2)e - 22E_i(1,1)e + 12 \approx -0.03468104$$

■

Problem 11 *(Gautschi, Ch.2, 8, pag.126)*
Approximate the circular arc γ given by the equation $y(t) = \sqrt{1-t^2}$, $0 \le t \le 1$ (see figure) by a straight line l in the least squares sense, using either the weight function $w(t) = (1-t^2)^{-1/2}$, $t \in [0,1]$ or $w(t) = 1$, $t \in [0,1]$. Where does l intersect the coordinate axes in these two cases?
(Point of information $\int_0^{\frac{\pi}{2}} \cos^2\theta d\theta = \frac{\pi}{4}$, $\int_0^{\frac{\pi}{2}} \cos^3\theta d\theta = \frac{2}{3}$).

Solution. The normal equations (first case)

$$(\varphi_0,\varphi_0)c_0 + (\varphi_0,\varphi_1)c_1 = (\varphi_0, y)$$

$$(\varphi_0,\varphi_1)c_1 + (\varphi_1,\varphi_1)c_1 = (\varphi_1, y)$$

or, using orthogonal polynomials

$$\varphi(t) = c_0\pi_0(t) + c_1\pi_1(t)$$

$$c_j = \frac{(y,\pi_j)}{(\pi_j,\pi_j)}$$

first case $w(t) = (1-t^2)^{-1/2}$

$$(\varphi_0,\varphi_0) = \int_0^1 (1-t^2)^{-1/2}dt = \arcsin t\Big|_0^1 = \frac{\pi}{2}$$

$$(\varphi_0, \varphi_1 = \int_0^1 \frac{t}{\sqrt{1-t^2}} dt = -\sqrt{1-t^2}\Big|_0^1 = 1$$

$$(\varphi_1, \varphi_1) = \int_0^1 \frac{t^2}{\sqrt{1-t^2}} dt = \int_0^{\pi} \frac{\sin^2\theta}{\cos\theta} \cos\theta dt = \int_0^{\frac{\pi}{2}} \frac{1-\cos 2\theta}{2} d\theta = \frac{\pi}{4}$$

$$(y, \varphi_0) = \int_0^1 \frac{1}{\sqrt{1-t^2}} \sqrt{1-t^2} dt = 1$$

$$(y, \varphi_1) = \int_0^1 \frac{t}{\sqrt{1-t^2}} \sqrt{1-t^2} dt = \frac{1}{2}$$

$$\begin{cases} \frac{\pi}{2} c_0 + c_1 = 1 \\ c_0 + \frac{\pi}{4} c_1 = \frac{1}{2} \end{cases}$$

$$\Delta = \frac{\pi^2}{8} - 1 = \Delta c_0 = \begin{vmatrix} 1 & 1 \\ \frac{1}{2} & \frac{\pi}{4} \end{vmatrix} = \frac{\pi}{4} - \frac{1}{2}$$

$$c_0 = \frac{\pi - 2}{4} \cdot \frac{8}{\pi^2 - 8} = \frac{2(\pi - 2)}{\pi^2 - 8}$$

$$\Delta c_1 = \begin{vmatrix} \frac{\pi}{2} & 1 \\ 1 & \frac{1}{2} \end{vmatrix} = \frac{\pi}{4} - 1$$

$$c_1 = \frac{\pi - 4}{4} \cdot \frac{8}{\pi^2 - 8} = \frac{2(\pi - 4)}{\pi^2 - 8}$$

$$\varphi(t) = \frac{2(\pi - 2)}{\pi^2 - 8} + \frac{2(\pi - 4)}{\pi^2 - 8} t$$

2nd case $w(t) = 1$

$$(\varphi_0, \varphi_0) = \int_0^1 dt = 1$$

$$(\varphi_0, \varphi_1) = \int_0^1 t dt = \frac{1}{2}$$

$$(\varphi_1, \varphi_1) = \int_0^1 t^2 dt = \frac{1}{3}$$

$$(y, \varphi_0) = \int_0^1 \sqrt{1-t^2} dt = \frac{\pi}{4}$$

$$(y, \varphi_1) = \int_0^1 t\sqrt{1-t^2} dt = \frac{1}{3}$$

$$\begin{cases} c_0 + \dfrac{1}{2}c_1 = \dfrac{\pi}{4} \\ \\ \dfrac{1}{2}c_0 + \dfrac{1}{3}c_1 = \dfrac{1}{3} \end{cases}$$

$$c_0 = \pi - 2, \quad c_1 = -\frac{3}{2}\pi + 4$$

$$\varphi(t) = \pi - 2 + \left(4 - \frac{3\pi}{2}\right)t$$

■

Problem 12 *(Gautschi, Ch.2, 9, pag.127)*

(a) Let the class ϕ_n approximating functions have the following properties. Each $\varphi \in \phi_n$ is defined on an interval $[a, b]$ symmetric with respect to the origin (i.e. $a = -b$), and $\varphi(t) \in \phi_n$ implies $\varphi(-t) \in \phi_n$. Let $d\lambda(t) = \omega(t)dt$, with $\omega(t)$ an even function on $[a, b]$ (i.e. $\omega(-t) = \omega(t)$). Show: if f is an even function on $[a, b]$ then so is its least squares approximant, $\widehat{\varphi}_n$, on $[a, b]$ from ϕ_n.

(b) Consider the "hat function"

$$f(t) = \begin{cases} 1 - t, & t \in [0, 1] \\ 1 + t, & t \in [-1, 0]. \end{cases}$$

Determine its least squares approximation on $[-1, 1]$ by a quadratic function. (Use $d\lambda(t) = dt$). Simplify your calculation by using part (a). Determine where the error vanishes.

Solution. (a) $t = -x$

$$D = \int_{-a}^{a} \omega(t)[f(t) - \widehat{\varphi}_n(t)]^2 dt \to \min$$

$$= -\int_{-a}^{a} \omega(-x)[f(-x) - \widehat{\varphi}_n(-x)]^2 dx$$

$$= \int_{-a}^{a} \omega(x)[f(x) - \widehat{\varphi}_n(-x)]^2 dx$$

so

$$\int_{-a}^{a} \omega(x)\{[f(x) - \varphi_n(x)]^2 - [f(x) - \varphi_n(-x)]^2\} = 0$$

$$\int_{-a}^{a} \omega(x)(f(x) - \widehat{\varphi}_n(x) - f(x) + \widehat{\varphi}_n(-x))(2f(x) - \varphi_n(x) + \varphi_n(x))dx = 0$$

$$\Rightarrow \widehat{\varphi}_n(x) - \widehat{\varphi}_n(-x) = 0 \Rightarrow \widehat{\varphi}_n(x) = \varphi_n(-x)$$

Another method

$$\pi_{-1}(t) = 0, \quad \pi_0(t) = 1$$

$$\pi_{k+1}(t) = t\pi_k(t) - \beta_k \pi_{k-1}(t)$$

$$\pi_1(t) = t$$

The roots of π_k are symmetric with respect to the origin.

$$\pi_k(-t) = \pi_k(t) \text{ for } k \text{ even}$$

$$\pi_k(-t) = -\pi_k(t) \text{ for } k \text{ odd}$$

$$\pi_{k+1}(-t) = -t\pi_k(-t) - \beta_k \pi_{k-1}(-t)$$

k even

$$\pi_{k+1}(-t) = t\pi_k(t) + \beta_k \pi_{k-1}(-t) = -\pi_{k+1}(t)$$

k odd

$$\pi_{k+1}(-t) = -t\pi_k(-t) - \beta_k \pi_{k-1}(-t) = -t\pi_k(t) - \beta_k \pi_{k-1}(t) = \pi_{k+1}(t)$$

(b) $\widehat{\varphi}_2(t) = c_0 l_0(t) + c_1 l_1(t) + c_2 l_2(t)$

$$l_0(t) = 1, \quad l_1(t) = t$$

$$l_2(t) = tl_1(t) - \beta_1 = t^2 - \frac{1}{3}$$

so $c_1 = 0$

$$c_0 = \frac{(f, l_0)}{(l_0, l_0)} = \frac{1}{2}$$

$$c_1 = 0$$

$$c_2 = \frac{(f, l_2)}{(l_2, l_2)} = \frac{-\frac{1}{6}}{\frac{8}{45}} = -\frac{1}{6} \cdot \frac{45}{8} = -\frac{15}{16}$$

$$\varphi_2(t) = \frac{1}{2} - \frac{15}{16}\left(t^2 - \frac{1}{3}\right)$$

Solving the equation $f(t) = \varphi_2(t)$ we obtain the solutions

$$t \in \left\{ \frac{8+\sqrt{19}}{15}, \frac{8-\sqrt{19}}{15}, \frac{-8+\sqrt{19}}{15}, \frac{-8-\sqrt{19}}{15} \right\}$$

■

Problem 13 (Gautschi, Ch.2, 15) *Let f be a given function on $[0,1]$ satisfying $f(0) = 0$, $f(1) = 1$.*

(a) Reduce the problem of approximating f on $[0,1]$ in the (continuous, equally weighted) least squares sense by a quadratic polynomial p satisfying $p(0) = 0$, $p(1) = 1$ to an unconstrained least squares problem (for a different function).

(b) Apply the result of (a) to $f(t) = t^r$, $r > 2$. Plot the approximation against the exact function for $r = 3$.

Solution.

$$p(x) = ax^2 + bx + c$$

$$p(0) = c = 0$$

$$p(1) = a + b = 1 \Rightarrow b = 1 - a$$

$$p(x) = ax^2 + (1-a)x$$

$$E^2[a] = \int_0^1 [f(x) - ax^2 - (1-a)x]^2 dx \to \min$$

$$E^2[a] = \int_0^1 [f(x) + x - a(x^2 - x)]^2 dx$$

$$\frac{\partial E^2}{\partial a} = -2\int_0^1 [f(x) + x - a(x^2 - x)](x^2 - x)dx = 0$$

$$a = 30\int_0^1 f(x)(x^2 - x)dx + \frac{5}{2}$$

(b) for $f(t) = t^r$

$$a = 30\int_0^1 t^{r+1}(t^2 - t)dt + \frac{5}{2} = \frac{5}{2} + \frac{30}{r+3} - \frac{30}{r+2}$$

for $r = 3$, $a = \frac{3}{2}$. ∎

Problem 14 (Gautschi, Ch.2, 60, pag.138) *Consider the problem of finding a polynomial $p \in \mathbb{P}_n$ such that*

$$p(x_0) = f(x_0), \quad p'(x_i) = f_i', \quad i = 1, 2, \ldots, n,$$

where x_i, $i = 1, 2, \ldots, n$ are distinct nodes. (It is not excluded that $x_1 = x_0$). This is neither a Lagrange nor a Hermite interpolation problem (why not?). Nevertheless, show that the problem has a unique solution and describe how it can be obtained. Find the rest.

Solution.

$$P(x) = a_0 + a_1 x + \cdots + a_n x^n$$
$$P'(x) = a_1 + 2a_2 x + \cdots + n a_n x^{n-1}$$
$$P(x_0) = a_0 + a_1 x_0 + \cdots + a_n x_0^n = f_0$$
$$P'(x_i) = a_1 + 2a_2 x_i + \cdots + n a_n x_i^{n-1} = f_i'$$

The determinant

$$\Delta = \begin{vmatrix} 1 & x_0 & x_0^2 & \dots & x_0^n \\ 0 & 1 & 2x_1 & \dots & nx_1^{n-1} \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 1 & 2x_n & \dots & nx_n^{n-1} \end{vmatrix}$$

$$= \begin{vmatrix} 1 & 2x_1 & \dots & nx_1^{n-1} \\ \dots & \dots & \dots & \dots \\ 1 & 2x_n & \dots & nx_n^{n-1} \end{vmatrix} = n! \begin{vmatrix} 1 & x_1 & \dots & x_1^{n-1} \\ \dots & \dots & \dots & \dots \\ 1 & x_n & \dots & x_n^{n-1} \end{vmatrix}$$
$$= n! V(x_1, \dots, x_n) \neq 0 \text{ if } x_i \neq x_j \ (i = j)$$

For the rest we use Peano's theorem.

$$(R_n f)(x) = \int_a^b K_n(x,t) f^{(n+1)}(t) dt$$

$$K_n(x,t) = \frac{1}{n!} \left[(x-t)_+^n - \sum_{i=0}^{n} a_i((x-t)_+^n) x^i \right]$$

■

Problem 15 (Gautschi, Ch.2, 56, pag.137) *Consider the data* $f(0) = 5,\ f(1) = 3,\ f(3) = 5,\ f(4) = 12$.

(a) *Use Newton's formula to obtain the appropriate interpolation polynomial* $L_3 f$.

(b) *The data suggest that* f *has a minimum between* $x = 1$ *and* $x = 3$. *Find an approximate value for the location* x_{min} *of the minimum.*

Solution.

$$\begin{array}{ccccc} 0 & 5 & -2 & 1 & \frac{1}{4} \\ 1 & 3 & 1 & 2 & \\ 3 & 5 & 7 & & \\ 4 & 12 & & & \end{array}$$

$$(L_3f)(x) = 5 - 2x + x(x-1) + \frac{1}{4}x(x-1)(x-3) = 5 - \frac{9}{4}x + \frac{1}{4}x^3$$

$$(L_3f)'(x) = -\frac{9}{4} + \frac{3}{4}x^2 = \frac{3}{4}(x^2-3)$$

$$x_{1,2} = \pm\sqrt{3}$$

$$\begin{array}{ccccc} & -\sqrt{3} & & \sqrt{3} & \\ \hline + & 0 & - & 0 & + \\ \nearrow & & \searrow & & \nearrow \end{array}$$

$$x_{min} \approx \sqrt{3}$$

$$f_{min} \approx (L_3f)(\sqrt{3}) = 5 - \frac{9\sqrt{3}}{4} + \frac{1}{4}\cdot 3\sqrt{3} = 5 - \frac{3\sqrt{3}}{2}$$

■

Problem 16 (Gautschi, Ch.2, 58, pag.137) *Suppose f is a function on $[0,3]$ for which one knows that*

$$f(0) = 1, \quad f(1) = 2, \quad f'(1) = -1, \quad f(3) = f'(3) = 0.$$

(a) Estimate $f(2)$ using Hermite interpolation.

(b) Estimate the maximum possible error of the answer given in (a) if one knows, in addition, that $f \in C^5[0,3]$ and $|f^{(5)}(x)| \le M$ on $[0,3]$. Express the answer in term of M.

Solution. The divide differences table is

	D^0	D^1	D^2	D^3	D^4
0	1	1	-2	$\frac{2}{3}$	$-\frac{5}{12}$
1	2	-1	0	$\frac{1}{4}$	
1	2	-1	$\frac{1}{2}$		
3	0	0			
3	0				

$$(H_4f)(x) = 1 + x - 2x(x-1) + \frac{2}{3}x(x-1)^2 - \frac{5}{12}x(x-1)^2(x-3)$$

$$(H_4f)(2) = 1 + 2 - 2\cdot 2\cdot 1 + \frac{2}{3}\cdot 2\cdot 1 - \frac{5}{12}\cdot 2\cdot 1(-1)$$

$$= 3 - 4 + \frac{4}{3} + \frac{10}{12} = -1 + \frac{4}{3} + \frac{5}{6} = \frac{7}{6}$$

$$(R_4 f)(x) = \frac{x(x-1)^2(x-3)^2}{4!} f^{(5)}(\xi)$$

$$|(R_3 f)(x)| \le \frac{1}{24}|x(x-1)^2(x-3)^2|M$$

$$\le \frac{1}{24}\left(\frac{6+\sqrt{21}}{5}\right)\left(\frac{1+\sqrt{21}}{5}\right)^2\left(\frac{-9+\sqrt{21}}{5}\right)^2$$

$$= \frac{1}{24\cdot 3125}(6+\sqrt{21})(1+\sqrt{21})^2(-9+\sqrt{21})^2 M$$

$$= \frac{1}{24\cdot 3125}(4896+336\sqrt{21})$$

$$= \frac{1}{75000}(4896+336\sqrt{21})M = \frac{204+14\sqrt{21}}{3125}M$$

■

Problem 17 ((Gautschi, Ch.2, 59, pag.137) *(a) Use Hermite interpolation to find a polynomial of lowest degree satisfying*

$$p(-1) = p'(-1) = 0, \quad p(0) = 1, \quad p(1) = p'(1) = 0.$$

Simplify your expression for p as much as possible.

(b) Suppose the polynomial p of (a) is used to approximate the function $f(x) = [\cos(\pi x/2)]^2$ *on* $-1 \le x \le 1$.

(b_1) *Express the error* $e(x) = f(x) - p(x)$ *(for some* fixed x *in* $[-1,1]$*) in terms of an appropriate derivative of* f.

(b_2) *Find an upper bound for* $|e(x)|$ *(still for a fixed* x *in* $[-1,1]$*).*

(b_3) *Estimate* $\max\limits_{-1\le x\le 1} |e(x)|$.

Solution.

	D^0	D^1	D^2	D^3	D^4
-1	0	0	1	-1	1
-1	0	1	-1	1	
0	1	-1	1		
1	0	0			
1	0				

(a) $(H_4 f)(x) = 0 + 0\cdot(x+1) + 1\cdot(x+1)^2 - 1\cdot x(x+1)^2 - 1\cdot x(x+1)^2(x-1)$

$= (x+1)^2 - x(x+1)^2 + x(x+1)^2(x-1) = (x+1)^2[1 - x + x(x-1)]$

$$= (x+1)^2[1 - x + x^2 - x] = (x+1)^2(x-1)^2$$

Remark. $x = -1$ and $x = 1$ are double roots of $H_4 f$ so

$$(H_4 f)(x) = c(x+1)^2(x-1)^2$$

$$(H_4 f)(0) = c = 1 \Rightarrow (H_4 f)(x) = (x+1)^2(x-1)^2$$

(b) (b_1) $(R_4 f)(x) = \dfrac{(x+1)^2 x(x-1)^2}{5!} f^{(5)}(\xi)$

$$= \frac{(x+1)^2 x(x-1)^2}{120}\left[-\pi^5 \cos\frac{\pi\xi}{2} \sin\frac{\pi\xi}{2}\right]$$

(b_2) $|(R_4 f)(x)| \le \dfrac{|x|(x+1)^2(x-1)^2}{120}\dfrac{\pi^5}{2}$

(b_3) $\|R_4 f\| \le \dfrac{16\sqrt{5}}{120 \cdot 125} \cdot \dfrac{\pi^5}{8} = \dfrac{\pi^5\sqrt{5}}{15 \cdot 125} = \dfrac{\pi^5\sqrt{5}}{1875}$ ■

Problem 18 (Gautschi, Ch.2, 61, pag.138) *Let*

$$f(t) = \begin{cases} 0 & \text{if} \quad 0 \le t \le \frac{1}{2} \\ 1 & \text{if} \quad \frac{1}{2} \le t \le 1 \end{cases}$$

(a) Find the linear least squares approximant $\widehat{p}_1$ to f on $[0,1]$, that is, the polynomial $p_1 \in \mathbf{P}_1$ for which

$$\int_0^1 [p_1(t) - f(t)]^2 dt = \min.$$

Use the normal equations with $\pi_0(t) = 1$, $\pi_1(t) = t$.

(b) Can you do better with continuous piecewise linear functions (relative to the partition $[0,1] = \left[0, \frac{1}{2}\right] \cup \left[\frac{1}{2}, 1\right]$)? Use the normal equations for the B-spline basis B_0, B_1, B_2.

Solution. (a) Normal equations

$$\begin{cases} (\pi_0, \pi_0)a + (\pi_0, \pi_1)b = (\pi_0, f) \\ (\pi_1, \pi_0)a + (\pi_1, \pi_1)b = (\pi_1, f) \end{cases}$$

i.e.

$$\begin{cases} a + \dfrac{1}{2}b = \dfrac{1}{2} \\[2ex] \dfrac{1}{2}a + \dfrac{1}{3}b = \dfrac{3}{8} \end{cases} \Rightarrow a = -\frac{1}{4},\ b = \frac{3}{2}$$

$$p_1(t) = -\frac{1}{4} + \frac{3}{2}t$$

(b)

$$B_0(t) = \begin{cases} 1 - 2t, & t \in \left[0, \frac{1}{2}\right] \\ 0, & \text{otherwise} \end{cases}$$

$$B_1(t) = \begin{cases} 2t, & t \in \left[0, \frac{1}{2}\right] \\ 2 - 2t, & t \in \left[\frac{1}{2}, 1]\right] \\ 0, & \text{otherwise} \end{cases}$$

$$B_2(t) = \begin{cases} -1 + 2t, & t \in \left[\frac{1}{2}, 1\right] \\ 0, & \text{otherwise} \end{cases}$$

$$s(t) = c_0 B_0(t) + c_1 B_1(t) + c_2 B_2(t)$$

Normal equations

$$(B_0, B_0)c_0 + (B_0, B_1)c_1 + (B_0, B_2)c_2 = (B_0, f)$$

$$(B_1, B_0)c_0 + (B_1, B_1)c_1 + (B_1, B_2)c_2 = (B_1, f)$$

$$(B_2, B_0)c_0 + (B_2, B_1)c_1 + (B_2, B_2)c_2 = (B_2, f)$$

or in matrix form

$$\begin{bmatrix} \frac{1}{6} & \frac{1}{12} & 0 \\ \frac{1}{12} & \frac{1}{3} & \frac{1}{12} \\ 0 & \frac{1}{12} & \frac{1}{6} \end{bmatrix} c = \begin{bmatrix} 0 \\ \frac{1}{4} \\ \frac{1}{4} \end{bmatrix}$$

with solution $c_0 = -\frac{1}{4}$, $c_1 = \frac{1}{2}$, $c_2 = \frac{5}{4}$

$$s(t) = \begin{cases} -\frac{1}{4} + \frac{3}{2}t, & t \in [0, 1] \\ 0, & \text{otherwise} \end{cases}$$

So, there is no difference. ■

Problem 19 *(Gautschi, Ch.2, 29, p.132)*
In a table of the Bessel functions

$$J_0(x) = \frac{1}{\pi}\int_0^\pi \cos(x\sin\theta)d\theta,$$

where x is incremented in steps of size h, how small must h be chosen if the table is to be "linearly interpolable" with an error less than 10^{-6} in absolute value?

Solution. $x_0 = x,\ x_1 = x+h$

$$J_0(t) \approx (L_1 J_0)(t; x_0, h_1)$$

The error is

$$(R_1 f)(t) = \frac{(t-x)(t-x-h)}{2!}J_0''(\xi)$$
$$|(R_1 f)(t)| \le \max_{t\in[x,x+h]} |(t-x)(t-x-h)| \max_{\xi\in(x,x+h)} J_0''(\xi)$$

But

$$J_0''(t) = \frac{1}{\pi}\int_0^\pi -\cos(x\sin\theta)\sin^2\theta dt$$
$$|J_0''(t)| \le \frac{1}{\pi}\int_0^\pi \sin^2\theta dt = \frac{1}{\pi}\cdot\frac{\pi}{2} = \frac{1}{2}$$

so $|J_0''(\xi)| \le \frac{1}{2}$, and

$$|(R_1 f)(t)| \le \frac{h^2}{8}\cdot\frac{1}{2} \le 10^{-6} \Rightarrow h^2 \le \frac{16}{100000} \Rightarrow h < \frac{1}{250} = 0.004$$

■

Problem 20 (Gautschi, Ch.2, 69, p.139) *Let*

$$s_1(x) = 1 + c(x+1)^3, \quad -1 \le x \le 0,$$

where c is a (real) parameter.
Determine $s_2(x)$ on $0 \le x \le 1$ so that

$$s(x) := \begin{cases} s_1(x) & \text{if } -1 \le x \le 0 \\ s_2(x) & \text{if } 0 \le x \le 1 \end{cases}$$

is a natural cubic spline on $[-1,1]$ with knots at $-1, 0, 1$. How c must be chosen if one wants $s(1) = -1$?

Solution. $s_2(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$
$s \in C^r[-1,1]$
$s_1(0) = s_2(0) \Rightarrow 1 + c = a_0$
$s_1'(0) = s_2'(0) \Rightarrow 3c = a_1$
$s_1''(0) = s_2''(0) \Rightarrow 6c = 2a_2$
$s_2''(1) = 2a_2 + 6a_3 = 0$

$$\begin{cases} a_0 = 1 + c \\ a_1 = a_2 = 3c \\ a_3 = -\dfrac{a_2}{3} = -c \end{cases}$$

$$s_2(x) = 1 + c + 3cx + 3cx^2 - cx^3$$

If $s_2(x) = -1$ we must have $1 + c + 6c - c = -1$
$6c = -2 \Rightarrow c = -\dfrac{1}{3}$ ■

Problem 21 (Gautschi, Ch.2, p.19, pag.130) *Given the recursion relation*

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k - \beta_k \pi_{k-1}(t), \;\; k = 0, 1, 2, \ldots$$

for the (monic) orthogonal polynomials $\{\pi_j(\cdot; d\lambda)\}$ *and defining* $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$ *show that* $\|\pi_k\|^2 = \beta_0 \beta_1 \ldots \beta_k$, $k = 0, 1, 2, \ldots$. *How you can exploit this in a practical implementation of least-squares approximation with respect to an orthogonal system?*

Solution.

$$\beta_k = \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})} = \frac{\|\pi_k\|^2}{\|\pi_{k-1}\|^2}$$

$$\|\pi_k\|^2 = \beta_k \|\pi_{k-1}\|^2 = \beta_k \beta_{k-1} \|\pi_{k-2}\|^2 = \beta_k \beta_{k-1} \ldots \beta_0$$

$$c_j = \frac{(f, \pi_k)}{(\pi_k, \pi_k)} = (\beta_0 \beta_1 \ldots \beta_k)^{-1} (f, \pi_k)$$

■

Problem 22 *Discuss uniqueness and nonuniqueness of the least squares approximant to a function* f *in the case of a discrete set* $T = \{t_1, t_2\}$ *(i.e.,* $N = 2$*) and* $\Phi_n = \mathbb{P}_{n-1}$ *(polynomials of degree* $n-1$*). In case of nonuniqueness, determine all solutions.*

Solution. Let the least squares approximant to f from $\mathbb{P}_{n-1}$ be $\widehat{p}_{n-1}$. We have

for $n = 1$**:** unique $\widehat{p}_0 \in \mathbb{P}_0$, namely $\widehat{p}_0 = \frac{1}{2}(f_1 + f_2)$;

for $n = 2$**:** unique $\widehat{p}_1 \in \mathbb{P}_1$, namely $\widehat{p}_1 = (L_1 f)\,(t; t_1, t_2)$;

for $n \geq 3$**:** infinitely many $\widehat{p}_{n-1} \in \mathbb{P}_{n-1}$, namely all polynomials $\widehat{p}_{n-1}$ that interpolate f at t_1 and t_2,

$$\widehat{p}_{n-1}(t) = \widehat{p}_1(t) + (t - t_1)(t - t_2)q_{n-3}(t),$$

where q_{n-3} is an arbitrary polynomial of degree $n - 3$.

■

Problem 23 *Approximate the circular quarter arc given by the equation* $y(t) = \sqrt{1 - t^2}$, $0 \leq t \leq 1$ *(see figure) by a straight line* ℓ *in the least squares sense, using either the weight function* $w(t) = \left(1 - t^2\right)^{-1/2}$, $0 \leq t \leq 1$, *or* $w(t) = 1$, $0 \leq t \leq 1$. *Where does* ℓ *intersect the coordinate axes in these two cases?*

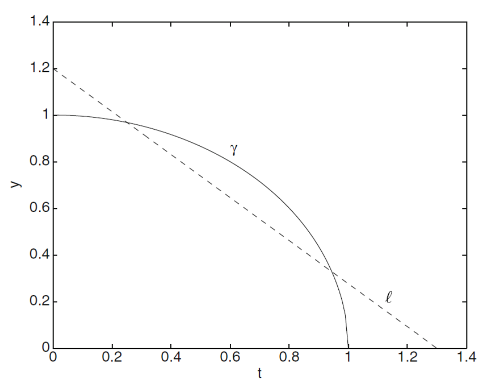

Figure 2.1: Problem 23

Solution. We let $\pi_0(t) = 1$, $\pi_1(t) = t$ and $f(t) = \sqrt{1 - t^2}$. Then, in the case $w(t)=(1-t^2)^{-1/2}$, we have, using the change of variables $t=\cos\theta$,

$$
\begin{aligned}
(\pi_0,\pi_0) &= \int_0^1 (1-t^2)^{-1/2}\mathrm{d}\,t = \frac{1}{2}\pi \\
(\pi_0,\pi_1) &= \int_0^1 t(1-t^2)^{-1/2}\mathrm{d}\,t = 1 \\
(\pi_1,\pi_1) &= \int_0^1 t^2(1-t^2)^{-1/2}\mathrm{d}\,t = \frac{1}{4}\pi \\
(\pi_0,f) &= \int_0^1 \mathrm{d}\,t = 1, \quad (\pi_1,f) = \int_0^1 t\mathrm{d}\,t = \frac{1}{2},
\end{aligned}
$$

so that the normal equations become

$$
\begin{aligned}
\frac{\pi}{2}c_0 + c_1 &= 1, \\
c_0 + \frac{\pi}{4}c_1 &= \frac{1}{2},
\end{aligned}
$$

and have the solution

$$c_0 = \frac{2\,(\pi-2)}{\pi^2-8} = 1.221\,2,\ c_1 = \frac{2\pi-8}{\pi^2-8} = -0.918\,28$$

In the case $w(t)=1$, we get :

$$
\begin{aligned}
(\pi_0,\pi_0) &= \int_0^1 \mathrm{d}\,t = 1,\ (\pi_0,\pi_1) = \int_0^1 t\mathrm{d}\,t = \frac{1}{2},\ (\pi_1,\pi_1) = \int_0^1 t^2\mathrm{d}\,t = \frac{1}{3} \\
(\pi_0,f) &= \int_0^1 (1-t^2)^{1/2}\mathrm{d}\,t = \frac{1}{4}\pi,\ (\pi_1,f) = \int_0^1 t(1-t^2)^{1/2}\mathrm{d}\,t = \frac{1}{3}.
\end{aligned}
$$

and the normal equations are

$$
\begin{aligned}
c_0 + \frac{1}{2}c_1 &= \frac{\pi}{4} \\
\frac{1}{2}c_0 + \frac{1}{3}c_1 &= \frac{1}{3}
\end{aligned}
$$

Solution is: $c_0 = \pi - 2 = 1.141\,6,\ c_1 = 4 - \frac{3}{2}\pi = -0.712\,39$

Thus, the line

$$\ell : y(t) = c_0 + c_1 t$$

intersects the y-axis at $y=c_0$ and the t-axis at $t=-c_0/c_1$. For the two weight functions, the values are respectively

$$
\begin{aligned}
&y = 1.2212...,\ t = 1.3298...\ \left(w(t) = (1-t^2)^{-1/2}\right); \\
&y = 1.1415...,\ t = 1.6024...\ (w(t) = 1).
\end{aligned}
$$

Thus, the weight function $(1-t^2)^{-1/2}$ forces the line ℓ to be steeper and intersect the t-axis closer to 1. ■

Problem 24 *Let*

$$\begin{cases} \pi_{k+1}(t) = (t-\alpha_k)\,\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, \ldots n-1 \\ \pi_{-1}(t) = 0, \ \pi_0(t) = 1 \end{cases} \tag{*}$$

and consider

$$p_n(t) = \sum_{j=0}^{n} c_j \pi_j(t).$$

*Show that p_n can be computed by the following algorithm (*Clenshaw's algorithm*):*

$$\begin{cases} u_n = c_n, \ u_{n+1} = 0; \\ u_k = (t-\alpha k)\,u_k + \beta_{k+1} u_{k+2} + c_k, \quad k = n-1, n-2, \ldots, 0. \\ p_n = u_{0.} \end{cases} \tag{**}$$

{Hint*: write * in matrix form in terms of the vector $\pi^T = [\pi_0, \pi_1, \ldots, \pi_n]$ and a unit triangular matrix. Do likewise for (**).*}

Solution. The relations (*) in matrix form are

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -(t-\alpha_0) & 1 & 0 & \cdots & 0 & 0 \\ \beta_1 & -(t-\alpha_1) & 1 & \cdots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \beta_{n-2} & -(t-\alpha_{n-2}) & 1 & 0 \\ 0 & 0 & 0 & \beta_{n-1} & -(t-\alpha_{n-1}) & 1 \end{bmatrix} \begin{bmatrix} \pi_0 \\ \pi_1 \\ \pi_2 \\ \vdots \\ \pi_{n-2} \\ \pi_{n-1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$$

that is,

$$L\pi = e_1, \quad e_1 = [1, 0, \ldots, 0]^T.$$

with L unit lower triangular, as shown. Likewise, the relations for the u_k in (**) are, in matrix form,

$$L^T u = c, \ u^T = [u_0, u_1, \ldots, u_n], \ c^T = [c_0, c_1, \ldots, c_n].$$

Therefore,

$$p_n = c^T \pi = u^T L \pi = u^T e_1 = u_0.$$

■

Problem 25 *Let $\Delta : a = x_1 < x_2 < x_3 < \cdots < x_{n-1} < x_n = b$ be a subdivision of [a, b] into $n-1$ subintervals. Suppose we are given values $f_i = f(x_i)$ of some function $f(x)$ at the points $x = x_i$, $i = 1, 2, \ldots, n$. In this problem $s \in \mathbb{S}_2^1$ is a quadratic spline in $C^1[a,b]$ that interpolates f on Δ, that is, $s(x_i) = f_i$, $i = 1, 2, \ldots, n$.*

(a) Explain why one expects an additional condition to be required in order to determine s uniquely.

(b) Define $m_i = s'(x_i)$, $i = 1, 2, \ldots, n-1$. Determine $p_i = s|_{[x_i, x_{i+1}]}$, $i = 1, 2, \ldots, n-1$, in terms of f_i, f_{i+1}, and m_i.

(c) Suppose one takes $m_1 = f'(a)$. (According to (a), this determines s uniquely.) Show how m_2, m_3, $\ldots$, m_{n-1} can be computed.

Solution.

(a) The $3(n-1)$ parameters available are subject to $2(n-2)+2$ conditions of interpolation and $n-2$ conditions for continuity of the first derivative. The degree of freedom, therefore, is $3(n-1) - 2(n-2) - 2 - (n-2) = 1$. Thus we need one additional condition to determine the spline uniquely.

(b) With the usual notation $\Delta x_i = x_{i+1} - x_i$, the appropriate table of divided differences, and the desired polynomial p_i, are

x	f	$\mathcal{D}^1$	$\mathcal{D}^2$
x_i	f_i	m_i	$\frac{m_i - f[x_i, x_{i+1}]}{\Delta x_i}$
x_i	f_i	$f[x_i, x_{i+1}]$	
x_{i+1}	f_{i+1}		

$$p_i(x) = f_i + m_i(x - x_i) + (x - x_i)^2 \frac{m_i - f[x_i, x_{i+1}]}{\Delta x_i}, \quad 1 \le i \le n-1.$$

(c) We want $p_i'(x_{i+1}) = m_{i+1}$, $i = 1, 2, \ldots, n-2$. Thus,

$$m_i + 2\Delta x_i \frac{m_i - f[x_i, x_{i+1}]}{\Delta x_i} = m_{i+1} \iff$$
$$m_i + 2f[x_i, x_{i+1}] - 2m_i = m_{i+1},$$

or

$$\begin{cases} m_1 = f'(a) \\ m_{i+1} = 2f[x_i, x_{i+1}] - m_i \quad i = 1, 2, \ldots, n-2 \end{cases}$$

■

Problem 26 *Suppose that knots* $\Delta : a = t_0 < t_1 < \cdots < t_n = b$ *have been specified; let the nodes be the points*

$$\tau_0 = t_0, \ \tau_{n+1} = t_n$$
$$\tau_i = \frac{1}{2}\left(t_i + t_{i-1}\right), \quad i = 1, \ldots, n.$$

Find a quadratic spline function $Q \in S_2^1(\Delta)$ *that has the given knots and takes prescribed values at the nodes:*

$$Q(\tau_i) = y_i, \quad i = 0, 1, \ldots, n.$$

Solution. Let $Q_i = Q|_{[t_i, t_{i+1}]}$ and $m_i = Q'(t_i)$. We look for Q_i of the form

$$Q_i(x) = y_{i+1} + c_{i,1}(x - \tau_{i+1}) + c_{i,2}(x - \tau_{i+1})^2. \tag{2.1}$$

We get $c_{i,1}$ and $c_{i,2}$ from the conditions $Q_i(\tau_{i+1}) = y_{i+1}$, $Q_i'(t_i) = m_i$, and $Q_i'(t_{i+1}) = m_{i+1}$.

The last two conditions lead to

$$c_{i,1} + 2c_{i,2}\frac{t_i - t_{i+1}}{2} = m_i$$
$$c_{i,1} + 2c_{i,2}\frac{t_{i+1} - t_i}{2} = m_{i+1}$$

Solution is:

$$c_{i,1} = \frac{1}{2}m_i + \frac{1}{2}m_{i+1}, \quad c_{i,2} = \frac{m_{i+1} - m_i}{2\left(t_{i+1} - t_i\right)}$$

Now

$$Q_i(x) = y_{i+1} + \frac{1}{2}\left(m_i + m_{i+1}\right)\left(x - \tau_{i+1}\right) + \frac{1}{2h_i}(m_{i+1} - m_i)(x - \tau_{i+1})^2, \tag{2.2}$$

where $h_i = x_{i+1} - x_i$. Imposing continuity conditions at the interior knots,

$$\lim_{x \to t_i^-} Q_{i-1}(x) = \lim_{x \to t_i^+} Q_i(x)$$

we obtain

$$h_{i-1}m_{i-1} + 3(h_{i-1} + h_i)m_i + h_i m_{i+1} = 8(y_{i+1} - y_i), \quad i = 1, \ldots, n-1. \tag{2.3}$$

The first and last interpolation conditions must also be imposed:

$$Q(\tau_0) = y_0, \qquad Q(\tau_{n+1}) = y_{n+1}.$$

These two equations lead to

$$\begin{aligned} 3h_0 m_0 + h_0 m_1 &= 8(y_1 - y_0) \\ h_{n-1} m_{n-1} + 3h_{n-1} m_n &= 8(y_{n+1} - y_n) \end{aligned}$$

The system of equations governing the vector $\mathbf{m} = [m_0, m_1, ..., m_n]^T$ then can be written in the matrix form

$$\begin{bmatrix} 3h_0 & h_0 & & & & \\ h_0 & 3\,(h_0 + h_1) & h_1 & & & \\ & h_1 & 3\,(h_1 + h_2) & h_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & h_{n-2} & 3\,(h_{n-2} + h_{n-1}) & h_{n-1} \\ & & & & h_{n-1} & 3h_{n-1} \end{bmatrix} \begin{bmatrix} m_0 \\ m_1 \\ m_2 \\ \vdots \\ m_{n-1} \\ m_n \end{bmatrix}$$
$$= 8 \begin{bmatrix} y_1 - y_0 \\ y_2 - y_1 \\ y_3 - y_2 \\ \vdots \\ y_n - y_{n-1} \\ y_{n+1} - y_n \end{bmatrix}.$$

This system of $n+1$ equations in $n+1$ unknowns is tridiagonal, symmetric and diagonal dominant. After the $\mathbf{m}$ vector has been obtained, values of $Q(x)$ can be computed from Equation (2.2). ■

Chapter 3

Numerical Derivation and Integration

Problem 27 (Gautschi, Ch.3, 1, pag.193) *(a) Write the Hermite's interpolation formula for $f \in C^4[-1,1]$ and nodes $x_0 = -1$ simple, $x_1 = 0$ double, and $x_2 = 1$ simple.*

(b) Determine a quadrature formula by integrating the previous formula step by step.

(c) Transforms the previous formula into a formula on $[a,b]$. Is this a well-known formula?

Solution. (a) Use divided difference (Powell's) method. The divided differences table is

$$
\begin{array}{cccll}
-1 & f(-1) & f(0)-f(-1) & f'(0)-f(0)+f(-1) & \dfrac{f(1)-2f'(0)-f(-1)}{2} \\
0 & f(0) & f'(0) & f(1)-f(0)-f'(0) & \\
0 & f(0) & f(1)-f(0) & & \\
1 & f(1) & & &
\end{array}
$$

$$
\begin{aligned}
(H_3 f)(x) &= f(-1) + (x+1)[f(0)-f(-1)] \\
&+ x(x+1)[f'(0)-f(0)+f(-1)] + x^2(x+1)\frac{f(1)-2f'(0)-f(-1)}{2} \\
&= \frac{x^2-x^3}{2}f(-1) + (1-x^2)f(0) + \frac{x^2(x+1)}{2}f(1) + (x-x^3)f'(0)
\end{aligned}
$$

$$
(R_3 f)(x) = \frac{(x+1)x^2(x-1)}{4!}f^{(4)}(\xi)
$$

(b) $$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} (H_3 f)(x)dx + \int_{-1}^{1} (R_3 f)(x)dx$$

$$= \frac{1}{3}[f(-1) + 4f(0) + f(1)] - \frac{1}{90} f^{(4)}(\xi)$$

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

$$= \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

■

Problem 28 *(Gautschi, Ch.3, 10, pag.193)*

Estimate the number of subinterval required to obtain $\int_0^1 e^{-x^2} dx$ *to 6 correct decimal places (absolute error* $\leq \frac{1}{2} \times 10^{-6}$*)*

(a) by means of trapezoidal rule,

(b) by means of the composite Simpson rule.

Solution.

$$R_{2,n}(f) = -\frac{(1-0)^3}{12n^2} \|f''\|_\infty$$

$$\|f''\|_\infty = 2$$

because

$$f''(x) = (4x^2 - 2)e^{-x^2}$$

$$f^{(4)}(x) = (16x^4 - 48x^2 + 12)e^{-x^2}$$

$$\|f^{(n)}\|_\infty = 12$$

$$\frac{1}{6n^2} < \frac{1}{2} 10^{-6} \Rightarrow 3n^2 > 1000$$

$$n > \left[\sqrt{\frac{1000}{3}}\right] + 1$$

$$n = 20$$

$$R_{4,n}(f) = -\frac{(b-a)^5}{2880n^4} \|f^{(4)}\|_\infty = \frac{1}{2880n^4} \cdot 12 = \frac{1}{240n^4} < \frac{1}{2} 10^{-6}$$

$$120n^4 > 1000000$$

$$n = \left[\sqrt[4]{\frac{105}{12}} \right] + 1$$

$$n = 11$$

■

Problem 29 *(Gautschi, Ch.3, 15, pag.193)*
(a) Construct a weighted Newton-Cotes formula

$$\int_0^1 f(x)x^\alpha dx = a_0 f(0) + a_1 f(1) + R(f), \ \alpha > -1.$$

Explain why the formula obtained makes good sense.
(b) Derive an expression for the error term $R(f)$ in terms of an appropriate derivative of f.
(c) From the formulae in (a) and (b) derive an approximate integration formula for $\int_0^h g(t)t^\alpha dt$ ($h > 0$ small), including an expression for the error term.

Solution. (a) Formula must be exact for $f(x) = 1$ and $f(x) = x$.
Since

$$\mu_0 = \int_0^1 x^\alpha dx, \quad \mu_1 = \int_0^1 x x^\alpha dx, \quad \alpha > -1$$

exists, the formula makes sense

$$f(x) = 1, \quad \int_0^1 x^\alpha dx = \frac{1}{\alpha + 1} = a_0 + a_1$$

$$f(x) = x, \quad \int_0^1 x x^\alpha dx = \frac{1}{\alpha + 2} = a_0 \cdot 0 + a_1 \cdot 1$$

$$a_1 = \frac{1}{\alpha + 2}, \quad a_0 = \frac{1}{a + 1} - \frac{1}{\alpha + 2} = \frac{1}{(\alpha + 1)(\alpha + 2)}$$

$dex = 1$ since

$$\int_0^1 x^2 x^\alpha dx = \frac{1}{3 + \alpha} \neq \frac{1}{(\alpha + 1)(\alpha + 2)} \cdot 0 + \frac{1}{\alpha + 2} \cdot 1$$

$$R(f) = \int_0^1 K_1(t) f''(t) dt$$

$$K_1(t) = \int_0^1 (x-t)_+ dx - \frac{1}{(\alpha+1)(\alpha+2)}(0-t)_+ - \frac{1}{\alpha+2}(1-t)_+$$

$$= \frac{(1-t)^2}{2} - \frac{1}{\alpha+2}(1-t) = (1-t)\left(\frac{1-t}{2} - \frac{1}{\alpha+2}\right)$$

$$= \frac{(1-t)(\alpha - \alpha t + 2 - 2t - x)}{2(\alpha+2)} = \frac{(1-t)(\alpha - (\alpha+2)t)}{2(\alpha+2)}$$

$$t = \frac{\alpha}{\alpha+2}$$

$$t = hx$$

$$\int_0^4 g(t) t^\alpha dt = \int_0^1 g(hx) h^\alpha x^\alpha dx$$

$$= h^\alpha \int_0^1 g(hx) x^\alpha dx = \frac{h^\alpha}{(\alpha+1)(\alpha+2)} g(0) + \frac{h^\alpha}{\alpha+2} f(h) + R(f)$$

$$= \frac{h^\alpha}{\alpha+2}\left(\frac{1}{\alpha+1} g(0) + g(h)\right) + R(f)$$

$$R(f) = h^\alpha \int_0^h K_1(t) f''(t) dt$$

$$K_1(t) = \int_0^h (x-ht)_+ dx - \frac{1}{(\alpha+2)(\alpha+1)}(0-t)_+ - \frac{1}{\alpha+2}(h-t)_+$$

$$= \frac{(h-t)^2}{2} - \frac{1}{\alpha+2}(h-t) = (h-t)\left(\frac{h-t}{2} - \frac{1}{\alpha+2}\right)$$

$$= \frac{(h-t)(\alpha h - \alpha t_2 h - 2t - 2)}{2(\alpha+2)} = \frac{(h-t)((-\alpha-2)t + (\alpha+2)h - 2)}{2(\alpha+2)}$$

■

Problem 30 (Gautschi, Ch.3, 30, pag.198) *Consider a quadrature formula of the type*

$$\int_0^\infty e^{-x} f(x) dx = af(0) + bf(c) + R(f)$$

(a) *Find a, b, c such that the formula has the degree of exactness $d = 2$. Can you identify the formula so obtained?(Hint $\Gamma(n+1) = n!$).*

(b) *Let $p_2(x) = (H_2 f)(x, 0, 2, 2)$ be the Hermite interpolation polynomial interpolating f at the (simple) point $x = 0$ and the double point $x = 2$. Determine $\int_0^\infty e^{-x} p_2(x) dx$ and compare with the result in (a).*

(c) Obtain the remainder $R(f)$ in the form

$$R(f) = const \cdot f'''(\xi), \quad \xi > 0.$$

Solution. (a) Formula must be exact for $1, x, x^2$

$$\int_0^\infty e^{-x}dx = \Gamma(1) = 1 = a + b$$

$$\int_0^\infty xe^{-x}dx = \Gamma(2) = 1 = a \cdot 0 + bc$$

$$\int_0^\infty x^2e^{-x}dx = \Gamma(3) = 2 = a \cdot 0^2 + bc^2$$

$$c = 2, \quad b = \frac{1}{2}, \quad a = \frac{1}{2}$$

$$\int_0^\infty e^{-x}f(x)dx = \frac{1}{2}[f(0) + f(2)] + R(f)$$

(b) $x_0 = 0,\ r_0 = 0$
$x_1 = 2,\ r_1 = 1$
The divided differences table is

$$\begin{array}{llcc}
0 & f(0) & \dfrac{f(2)-f(0)}{2} & \dfrac{2f'(2)-f(2)+f(0)}{4} \\
2 & f(2) & f'(2) & \\
2 & f(2) & &
\end{array}$$

$$(H_2f)(x; 0, 2, 2) = f(0) + x\frac{f(2) - f(0)}{2} + x(x-2)\frac{2f'(2) - f(2) + f(0)}{4}$$

$$\int_0^\infty (H_2f)(x)e^{-x}dx = f(0) + \frac{1}{2}[f(2) - f(0)] = \frac{1}{2}[f(2) + f(0)]$$

$$R(f) = \int_0^\infty (R_2f)(x)e^{-x}dx$$

where R_2f is the Hermite remainder

$$R(f) = \int_0^\infty \frac{x(x-2)^x}{3!}e^{-x}f'''(\xi)dx$$

$$= \frac{1}{3!}f'''(\xi)\int_0^\infty x(x-2)^2e^{-x}dx$$

$$= \frac{1}{6}f'''(\xi)\int_0^\infty (x^3 - 4x^2 + 4x)e^{-x}dx = \frac{1}{6}f'''(\xi)[6 - 8 + 4] = \frac{1}{3}f'''(\xi)$$

■

Problem 31 *(Gautschi, 48, Ch.4, p.202)*

Assume, in Simpson's rule

$$\int_{-1}^{1} f(x)dx = \frac{1}{3}[f(-1) + 4f(0) + f(1)] + R(f)$$

that f is only of class $C^2[-1,1]$ instead of class $C^4[-1,1]$ as normally assumed.

(a) Find an error estimate

$$|R(f)| \leq const \cdot \|f''\|_\infty$$

(Hint. Apply Peano's theorem.)

(b) Transform the result in (a) to obtain Simpson's formula, with remainder estimate, for the integral

$$\int_{c-h}^{c+h} g(t)dt, \quad g \in C^2[c-h, c+h].$$

Solution.

$$R(f) = \int_{-1}^{1} K_1(t)d''(t)dt$$

$$\begin{aligned} K_2(t) &= \int_{-1}^{1} (x-t)_+ dx - \frac{1}{3}[(-1-t)_+ + 4(0-t)_+ + (1-t)_+] \\ &= \frac{(1-t)^2}{2} - \frac{1}{3}[4(0-t)_+ + (1-t)] \\ &= \begin{cases} \dfrac{(1-t)^2}{2} - \dfrac{1}{3}(1-t), & t \in [0,1] \\[2ex] \dfrac{(1-t)^2}{2} - \dfrac{1}{3}[4t + (1-t)], & t \in [-1,0] \end{cases} \end{aligned}$$

$t \in [0,1]$

$$K_1(t) = (1-t)\left[\frac{1-t}{2} - \frac{1}{3}\right] = \frac{(1-t)(3-3t-2)}{6} = \frac{(1-t)(1-3t)}{6}$$

$t \in \left[0, \frac{1}{3}\right]$, $K_1(t) > 0$

$t \in \left[\frac{1}{3}, 1\right]$, $K_1(t) < 0$

$t \in [-1, 0]$

$$K_1(t) = \frac{(1-t)^2}{2} - \frac{1}{3}[3t+1] = \frac{3-6t+3t^2-6t-2}{6} = \frac{3t^2-12t+1}{6}$$

$$\frac{(1-t)^2}{2} - \frac{1}{3}[(-1-t)_+ + 4(0-t)_+ + (1-t)_+] = \frac{(1-t)^2}{2} - \frac{1}{3}[4(0-t)_+ + (1-t)]$$

K_1 change its sign

$$|R(f)| \le \|f''\|_\infty \int_{-1}^{1} |K_1(t)| dt$$

$t \in [0, 1]$

$$\int_{-1}^{1} \frac{|1-t||1-3t|}{6} dt = \frac{4}{81}$$

$$\frac{1}{6}\int_{-1}^{0} |3t^2 - 12t + 1| dt = \frac{4}{3}$$

$$\int_{-1}^{1} |K_1(t)| dt = \frac{4}{81} + \frac{4}{3} = \frac{4}{3}\left(\frac{1}{27} + 1\right) = \frac{4 \cdot 28}{81} = \frac{112}{81}$$

(b) $\displaystyle\int_{c-h}^{c+h} g(t)dt = h\int_{-1}^{1} g(hx+c)dx$

$$= \frac{h}{3}[f(c-h) + 4f(c) + f(c+h)] + R(f)$$

$$|R(f)| \le \frac{h}{3} \cdot \frac{112}{81} \|f''\|_\infty$$

■

Problem 32 (Gautschi, 24, Ch.3, pag.197) *(a) Determine by Newton's interpolation formula the quadratic polynomial p interpolating f at $x = 0$ and $x = 1$ and f' at $x = 0$. Also express the error term of an appropriate derivative (assume continuous on $[0, 1]$).*

(b) Based on result of (a), derive an integration formula of the type

$$\int_0^1 f(x)dx = a_0 f(0) + a_1 f(1) + b_0 f'(0) + R(f)$$

Determine a_0, a_1, b_0 and an appropriate expression for $R(f)$.

(c) Transform the result of (b) to obtain an integration rule, with remainder, for $\int_c^{c+h} y(t)dt$*, where* $h > 0$*. (Do not rederive this rule from scratch).*

Solution. (a) divided difference-table

$$\begin{array}{llll} 0 & f(0) & f'(0) & f(1)-f(0)-f'(0) \\ 0 & f(0) & f(1)-f(0) & \\ 1 & f(1) & & \end{array}$$

$$(H_2 f)(x) = f(0) + xf'(0) + x^2[f(1) - f(0) - f'(0)]$$

$$= (1-x^2)f(0) + x^2 f(1) + (x - x^2)f'(0)$$

$$(R_2 f)(x) = \frac{x^2(x-1)}{3!} f'''(\xi)$$

(b) $a_0 = \int_0^1 (1-x^2)dx = \frac{2}{3}$

$$a_1 = \int_0^1 x^2 dx = \frac{1}{3}$$

$$b_0 = \int_0^1 (x - x^2)dx = \frac{1}{6}$$

$$(R_2 f)(x) = \int_0^1 \frac{x^2(x-1)}{3!} f'''(\xi)dx = \frac{f'''(\xi)}{3!} \int_0^1 x^2(x-1)dx$$

since $x^2(x-1) < 0$

$$= -\frac{1}{72} f'''(\xi)$$

(c) $\int_c^{c+h} y(x)dx = h \int_0^1 y(th_c)dt$

$$= h\left(\frac{2}{3}y(c) + \frac{1}{3}y(h+c) + \frac{h}{6}y'(c) - \frac{1}{72}y'''(h\xi + c)\right)$$

$$= \frac{2h}{3}y(c) + \frac{h}{3}y(h+c) + \frac{h^2}{6}y'(c) - \frac{h^4}{72}y'''(y)$$

■

Problem 33 *(Gautschi, Ch.3, 43, p.201)*

(a) Determine the quadratic spline $s_2(x)$ on $[-1,1]$ with a single knot at $x=0$ and such that $s_2(x)=0$ on $[-1,0]$ and $s_2(1)=1$.

(b) Consider a function $s(x)$ of the form

$$s(x) = c_0 + c_1 x + c_2 x^2 + c_3 s_2(x), \quad c_i = const$$

where $s_2(x)$ is as defined in (a). What kind of functions is s? Determine s such that

$$s(-1) = f_{-1}, \quad s(0) = f_0, \quad s'(0) = f_0', \quad s(1) = f_1$$

where $f_i = f(i)$, $f_i' = f'(i)$, $i = -1, 0, 1$.

(c) What quadrature rule does one obtain if one approximates $\int_{-1}^{1} f(x)dx$ by $\int_{-1}^{1} s(x)dx$, with s as obtained in (b)?

Solution. $s_2(x)|_{[0,1]} = a + bx + cx^2$

$$s_2(0) = a = 0, \quad s_2(1) = b + c = 1$$

$$s_2'(x) = b + 2cx, \quad s_2'(0) = b = 0$$

$$s_2(x) = \begin{cases} 0, & x \in [-1,0] \\ x^2, & x \in [0,1] \end{cases}$$

$$s(x) = c_0 + c_1 x + c_2 x^2 + c_3 s_2(x)$$

$$s(-1) = c_0 - c_1 + c_2 = f_{-1}$$

$$s(0) = c_0 = f_0$$

$$s'(1) = c_1 + 2c_2 x + c_3 s_2'(x)$$

$$s'(0) = c_1 = f'(0)$$

$$s(1) = c_0 + c_1 + c_2 + c_3 = f_1$$

$$c_0 = f_0, \quad c_1 = f_0', \quad c_2 = f_{-1} - f_0 + f_0'$$

$$c_3 = f_1 - 2f_0' - f_{-1}$$

$$s(x) = f_0 + f_0' x + (f_{-1} - f_0 + f_0')x^2 + (f_1 - 2f_0' - f_{-1})s_2(x)$$

$$\int_{-1}^{1} s(x)dx = 2f_0 + f_0' + \frac{2}{3}(f_{-1} - f_0 + f_0') + \frac{1}{3}(f_1 - 2f_0' - f_{-1})$$

$$= \frac{1}{3}f_{-1} + \frac{4}{3}f_0 + \frac{1}{3}f_1$$

(Simpson) ■

Problem 34 *(Gautschi, Ch.3, 15, pag.154)*

(a) Construct the weighted Newton-Cotes formula

$$\int_0^1 f(x)x^\alpha dx = a_0 f(0) + a_1 f(1) + R(f), \quad \alpha > -1.$$

Explain why the formula obtained makes good sense.

(b) Derive an expression for the error term $R(f)$ in terms of an appropriate derivative of f.

(c) From the formulae in (a) and (b) derive an approximate integration formula for $\int_0^h g(t)t^\alpha dt$ ($h > 0$ small), including an expression for the error term.

Solution. $f = 1$

$$a_0 + a_1 = \int_0^1 x^\alpha dx - \frac{1}{\alpha+1}, \quad dex = 1$$

$$a_0 \cdot 0 + a_1 \cdot 1 = \int_0^1 x^{\alpha+1} dx = \frac{1}{\alpha+2}$$

$$a_1 = \frac{1}{\alpha+2}$$

$$a_0 = \frac{1}{\alpha+1} - \frac{1}{\alpha+2} = \frac{1}{(\alpha+1)(\alpha+2)}$$

b) $R(f) = \int_0^1 K(t) f''(t) dt$

$$K(t) = \int_0^1 x^\alpha (x-t)_+ dx - \frac{1}{(\alpha+1)(\alpha+2)} \frac{(0-t)_+}{0} - \frac{1}{\alpha+1}(1-t)_+$$

$$= \int_t^1 x^\alpha (x-t) dx - \frac{1}{\alpha+1}(1-t)$$

$$= \frac{x^{\alpha+2}}{\alpha+2}\Big|_t^1 - \frac{x^{\alpha+1}t}{\alpha+1}\Big|_t^1 - \frac{1}{\alpha+1}(1-t)$$

$$= \frac{1-t^{\alpha+2}}{\alpha+2} - \frac{t-t^{\alpha+2}}{\alpha+1} - \frac{1}{\alpha+1}(1-t) = \frac{-1-t^{\alpha+2}}{(\alpha+1)(\alpha+2)} \leq 0$$

$$R(f) = \frac{1}{2!} f''(\xi) R(e_2)$$

$$= \frac{1}{2}\left[\int_0^1 x^{\alpha+2}dx - \frac{1}{(\alpha+1)(\alpha+2)}\cdot 0^2 - \frac{1}{\alpha+1}\right] f''(\xi)$$

$$= -\frac{1}{(\alpha+1)(\alpha+3)} f''(\xi)$$

(c) $\displaystyle\int_0^h g(t)t^\alpha dt = \int_0^1 g(hx)h^\alpha x^\alpha h dx$

$$= h^{\alpha+1}\int_0^1 g(hx)x^\alpha dx$$

$$= h^{\alpha+1}\left[\frac{1}{(\alpha+1)(\alpha+2)}g(0) + \frac{1}{\alpha+2}g(h)\right] - \frac{h^2}{(\alpha+1)(\alpha+2)}f''(\xi)$$

■

Problem 35 (Gautschi, Ch.3, 53, pag.203) *(a) Consider a quadrature formula of the type*

$$\int_0^1 f(x)dx = \alpha f(x_1) + \beta[f(1) - f(0)] + R(f) \tag{3.1}$$

and determine α, β, x_1 such that the degree of exactness is as large as possible. What is the maximum degree attainable?

(b) Use interpolation theory and the Peano Theorem to obtain a bound on $|R(f)|$ in terms of $\|f^{(r)}\|_\infty = \max\limits_{0\le x\le 1} |f^{(r)}(x)|$ for some suitable r.

(c) Adapt (*) including the bound on $|R(f)|$, to an integral of the form $\displaystyle\int_c^{c+h} f(t)dt$, where c is some constant and $h > 0$.

(d) Apply the result of (c) to develop a composite quadrature rule for $\displaystyle\int_a^b f(t)dt$ by subdividing $[a, b]$ into n subintervals of total length $h = \dfrac{b-a}{n}$. Find a bound for the total error.

Solution. (a) Formula must be exact for $f = 1, x, x^2, \ldots$

$$\int_0^1 dx = 1 = \alpha$$

$$\left.\begin{aligned}\int_0^1 x dx = \frac{1}{2} = x_1 + \beta \\ \int_0^1 x^2 dx = \frac{1}{3} = x_1^2 + \beta\end{aligned}\right\} \Rightarrow x_1 = \frac{1}{2} \pm \frac{\sqrt{3}}{6}$$

$$\beta = \pm\frac{\sqrt{3}}{6}$$

Since

$$\int_0^1 x^3 dx = \frac{1}{4} = x_1^3 + \beta = \left(\frac{1}{2} \pm \frac{\sqrt{3}}{6}\right)^3 \pm \frac{\sqrt{3}}{6} = \frac{1}{4} \pm \frac{11\sqrt{3}}{36},$$

the maximum degree of exactness is $r = 2$.

(b) $R(f) = \int_a^b K(t) f'''(t) dt$ where

$$K(t) = \frac{1}{2}\left\{\frac{(1-t)^3}{3} - \left(\frac{1}{2} \pm \frac{\sqrt{3}}{6} - t\right)_+^2 \mp \frac{\sqrt{3}}{6}[(1-t)_+^2 - (0-t)_+^2]\right\}$$

$$= \frac{1}{2}\begin{cases} \dfrac{(1-t)^3}{3} - \left(\dfrac{1}{2} \pm \dfrac{\sqrt{3}}{6} - t\right)^2 \mp \dfrac{\sqrt{3}}{6}(1-t)^2, \ t \in \left[0, \dfrac{1}{2} \pm \dfrac{\sqrt{3}}{6}\right] \\ \dfrac{(1-t)^3}{3} \pm \dfrac{\sqrt{3}}{6}(1-t)^2 \end{cases}$$

For $x_1 = \frac{1}{2} + \frac{\sqrt{3}}{6}$, $\beta = \frac{\sqrt{3}}{6}$, $K(t) \geq 0$.
For $x_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}$, $\beta = -\frac{\sqrt{3}}{6}$, $K(t) \leq 0$.
So, Peano's kernel preserve its sign.

$$R(f) = \frac{1}{3!} f''(\xi) R(e_3)$$

$$R(e_3) = \int_0^1 x^3 dx - x_1^3 - \beta(1^3 - 0^3) = \begin{cases} \dfrac{\sqrt{3}}{6} \\ -\dfrac{\sqrt{3}}{6} \end{cases}$$

$$R(f) = \pm\frac{\sqrt{3}}{216} f'''(\xi)$$

$$\int_0^1 f(x)dx = f(x_1) + \beta[f(1) - f(0)] \pm \frac{\sqrt{3}}{216} f'''(\xi)$$

(c) $t = hx + c$

$$\int_c^{c+h} f(t)dx = \int_0^1 f(c + hx)hdx$$

$$= h\{f(c + hx_1) + \beta[f(c + h) - f(c)]\} \pm \frac{\sqrt{3}}{216} h^4 f'''(\xi)$$

(d) $t_k = a + kh$, $h = \dfrac{b-a}{n}$

$$\int_a^b f(x)dx = \sum_{k=0}^{n-1} \int_{t_k}^{t_k+h} f(x)dx$$

$$= \sum_{k=0}^{n-1} h\{f(t_k + hx_1) + \beta[f(t_k + h) - f(t_k)]\} \pm \frac{\sqrt{3}}{210} h^4 \sum_{k=0}^{n-1} f'''(\xi)$$

$$= \beta[f(b) - f(a)] + h \sum_{k=0}^{n-1} f(t_k + hx_1) \pm \frac{\sqrt{3}}{216} \frac{(b-a)^4}{n^3} f'''(\xi)$$

■

Problem 36 *Find a Q.F. of the form*

$$\int_0^1 \frac{1}{\sqrt{x}} f(x)dx = af(0) + bf(x_1) + R(f)$$

that have a maximum degree of exactness.

Solution. I.

$$\mu_0 = \int_0^1 \frac{1}{\sqrt{x}} dx = \int_0^1 x^{-\frac{1}{2}} dx = \left. \frac{x^{\frac{1}{2}}}{\frac{1}{2}} \right|_0^1 = 2 = a + b$$

$$\mu_1 = \int_0^1 \frac{x}{\sqrt{x}} dx = \int_0^1 x^{\frac{1}{2}} dx = \frac{2}{3} = a \cdot 0 + bx_1$$

$$\mu_2 = \int_0^1 \frac{x^2}{\sqrt{x}} dx = \int_0^1 x^{\frac{3}{2}} dx = \frac{2}{5} = a \cdot 0 + bx_1^2$$

$$x_1 = \frac{2}{5} \cdot \frac{3}{2} = \frac{3}{5}$$

$$b \cdot \frac{3}{5} = \frac{2}{3}$$

$$b = \frac{10}{9}$$

$$a = \frac{8}{9}$$

$$\int_0^1 \frac{1}{\sqrt{x}} f(x)dx = \frac{8}{9} f(0) + \frac{10}{9} f\left(\frac{3}{5}\right) + R(f)$$

$$R(f) = \int_0^1 K(t) f'''(t)dt$$

$$K(t) = \frac{1}{2!}\left[\int_0^1 \sqrt{x}(x-t)_+^2 dx - \frac{8}{9}(0-t)_+^2 - \frac{10}{9}\left(\frac{3}{5}-t\right)_+^2\right]$$

$$= \frac{1}{2!}\left[\int_t^1 \sqrt{x}(x-t)^2 dx - \frac{10}{9}\left(\frac{3}{5}-t\right)_+^2\right] dx$$

$$K(t) \geq 0$$

because

$$K(t) = \frac{1}{2!}\begin{cases} \dfrac{6-20t+30t^2}{15}, & t \in \left(\dfrac{3}{5}, 1\right] \\[2ex] \dfrac{440t^2}{225}, & t \in \left[0, \dfrac{3}{5}\right] \end{cases}$$

Peano's Th. corollary $\Rightarrow$

$$R(f) = \frac{1}{3!} f'''(\xi) R(e_3)$$

$$R(e_3) = \int_0^1 \frac{1}{\sqrt{x}} x^3 dx - \frac{8}{9} \cdot 0^3 + \frac{10}{9} \cdot \frac{3^3}{5^3} = \frac{2}{7} - \frac{6}{25} = \frac{8}{175}$$

$$R(f) = \frac{1}{6} \cdot \frac{8}{175} f'''(\xi) = \frac{4}{525} f'''(\xi)$$

II. π_1 is orthogonal on $[-1, 1]$ with respect to

$$\omega(x) = x\omega(x) = x\frac{1}{\sqrt{x}} = \sqrt{x}$$

$$\int_0^1 \sqrt{x}(x-x_1)dx = \frac{2}{5} - \frac{2}{3}x_1 = 0, \quad x_1 = \frac{3}{5}$$

$$R(f) = \frac{f'''(\xi)}{3!}\int_0^1 \sqrt{x}\left(x-\frac{3}{5}\right)^2 dx$$

$$= \frac{f'''(\xi)}{3!}\left[\frac{2}{7} - \frac{6}{5}\cdot\frac{2}{5} + \frac{9}{25}\cdot\frac{2}{3}\right] = \frac{1}{6}\cdot\frac{8}{175}f'''(\xi) = \frac{4}{525}f'''(\xi)$$

■

Problem 37 *Find a Quadrature formula of the form*

$$\int_0^1 \sqrt{x}f(x)dx = af(0) + bf(x_1) + R(f)$$

that have a maximum degree of exactness.

Solution. I.

$$\int_0^1 \sqrt{x}dx = \frac{2}{3} = a + b$$

$$\int_0^1 x\sqrt{x}dx = \frac{2}{5} = a\cdot 0 + bx \Rightarrow x_1 = \frac{2}{7}\cdot\frac{5}{2} = \frac{5}{7}$$

$$\int_0^1 x^2\sqrt{x}dx = \frac{2}{7} = a\cdot 0 + bx_1^2$$

$$b = \frac{14}{25}, \quad a = \frac{8}{75}$$

$$K(t) \geq 0, \quad R(f) = \int_0^1 K(t)f'''(t)dt$$

$$R(f) = \frac{1}{3!}f'''(\xi)R(e_3)$$

$$R(e_3) = \int_0^1 \sqrt{x}x^3dx - \frac{8}{75}\cdot 0^3 - \frac{14}{25}\left(\frac{5}{7}\right)^3$$

$$= \frac{2}{9} - \frac{14}{25}\cdot\frac{5^3}{7^3} = \frac{2}{9} - \frac{10}{49} = \frac{8}{441}$$

$$R(f) = \frac{1}{2\cdot 3}\cdot\frac{8}{441}f'''(\xi) = \frac{4}{1323}f'''(\xi)$$

II. $\omega(x) = x\sqrt{x} = x^{\frac{3}{2}}$

$$\int_0^1 x^{\frac{3}{2}}(x-x_1)dx = \frac{2}{7} - \frac{2}{5}x_1 = 0, \quad x_1 = \frac{5}{7}$$

$$\begin{cases} a+b = \dfrac{2}{3} \\ \\ bx_1 = \dfrac{2}{5} \end{cases}$$

$$a = \frac{8}{75}, \quad b = \frac{14}{25}$$

$$R(f) = \frac{f'''(\xi)}{3!}\int_0^1 x\sqrt{x}\left(x-\frac{5}{7}\right)^2 dx = \frac{4}{1323}f'''(\xi)$$

■

Problem 38 (Gautschi, Ch.3, 50, pag.203) *(a) Use the method of undetermined coefficients to construct a quadrature formula of type*

$$\int_0^1 f(x)dx = af(0) + bf(1) + cf''(\gamma) + R(f)$$

having a maximum degree of exactness d, the variables being a, b, c and γ.

(b) Show that the Peano kernel Kd for the formula obtained in (a) is definite and hence express the remainder in the form

$$R(f) = e_{d+1}f^{(d+1)}(\xi), \quad 0 < \xi < 1.$$

Solution. (a) $a + b = \int_0^1 dx = 1$

$$a\cdot 0 + b\cdot 1 + c\cdot 0 = \int_0^1 xdx = \frac{1}{2}$$

$$a\cdot 0^2 + b\cdot 1^2 + 2c = \int_0^1 x^2dx = \frac{1}{3}$$

$$a\cdot 0^3 + b\cdot 1^2 + 6c\gamma = \frac{1}{4}$$

$$a = \frac{1}{2}, \quad b = \frac{1}{2}, \quad c = -\frac{1}{12}, \quad \gamma = \frac{1}{2}$$

$$\int_0^1 f(x)dx = af(0) + bf(1) - \frac{1}{12}f''\left(\frac{1}{2}\right) + R(f)$$

Since

$$\int_0^1 x^4dx = \frac{1}{5} \neq a\cdot 0^4 + b\cdot 1^4 - \frac{1}{12}\cdot 12\left(\frac{1}{2}\right)^2 = \frac{1}{4}$$

$d = 3$

(b) $R(f) = \int_0^1 K(t) f^{(4)}(t)dt$

$$K(t) = \frac{1}{4!}\left\{\int_0^1 (x-t)_+^3 dx - \frac{1}{2}(0-t)_+^3 - \frac{1}{2}(1-t)_+^3 + \frac{1}{12}\left[\left(\frac{1}{2}-t\right)_+^3\right]''\right\}$$

$$= \frac{1}{4!}\begin{cases} \frac{1}{4}t^4 - \frac{1}{2}t^3 = \frac{1}{4}t^3(t-2), & t \in \left[0, \frac{1}{2}\right) \\ \frac{t^4 - 2t^3 + 2t - 1}{4}, & t \in \left[\frac{1}{2}, 1\right] \end{cases}$$

$$K(t) \leq 0$$

$$R(f) = \frac{1}{4!}R(e_4) f^{(4)}(\xi) = -\frac{1}{480} f^{(4)}(\xi)$$

■

Problem 39 (Gautschi, Ch.3, 51, pag.203) *(a) Use the method of undetermined coefficient to construct a quadrature formula of the type*

$$\int_0^1 f(x)dx = -\alpha f'(0) + \beta f\left(\frac{1}{2}\right) + \alpha f'(1) + R(f)$$

that has a maximum degree of exactness.

(b) What is the precise degree of exactness of the formula obtained in (a)?

(c) Use the Peano kernel of the error functional Q to express $R(f)$ in terms of the appropriate derivative reflecting the result of (b).

(d) Transform the formula in (a) to one that is appropriate to evaluate $\int_c^{c+h} g(t)dt$ and then obtain the corresponding composite formula for $\int_a^b g(t)dt$, using n subintervals of equal length, and derive an error term. Interpret your result.

Solution. (a) $\int_0^1 dx = 1 = \beta$

$$\int_0^1 x dx = \frac{1}{2} = -\alpha + \frac{1}{2} + \alpha$$

$$\int_0^1 x^2 dx = \frac{1}{3} = -\alpha(2\cdot 0) + \frac{1}{4} + \alpha(2\cdot 1) = 2\alpha + \frac{1}{4}$$

$$\alpha = \frac{1}{24}$$

$$\int_0^1 f(x)dx = -\frac{1}{24}f'(0) + f\left(\frac{1}{2}\right) + \frac{1}{24}f'(1) + R(f)$$

(b) $dex = 3$

(c) $R(f) = \int_a^b K(t)f^{(4)}(t)dt$

$$K(t) = \frac{1}{3!}R[(x-t)_+^3]$$

$$R[(x-t)_+^3] = \int_0^1 (x-t)_+^3 dx + \frac{1}{24}[(0-t)_+^3] - \left(\frac{1}{2}-t\right)_+^3 - \frac{1}{24}[(1-t)_+^3]'$$

$$= \frac{(1-t)^4}{4} - \left(\frac{1}{2}-t\right)_+^3 - \frac{1}{8}(1-t)^2$$

$$= \begin{cases} \dfrac{(1-t)^4}{4} - \dfrac{1}{8}(1-t)^2, & t \in \left[\dfrac{1}{2}, 1\right] \\ \dfrac{(1-t)^4}{4} - \left(\dfrac{1}{2}-t\right)^3 - \dfrac{1}{8}(1-t)^2, & t \in \left[0, \dfrac{1}{2}\right] \end{cases}$$

Since $K(t) \geq 0$

$$R(f) = \frac{1}{4!}f^(4)(\xi)R(e4) = -\frac{7}{5760}f^{(4)}(\xi)$$

(d) $x = ht + c$, $dx = hdt$

$$\int_c^{c+h} g(x)dx = \int_0^1 g(ht+c)hdt = h\int_0^1 g(ht+c)$$

$$h\left[-\frac{1}{24}g'(c) + g\left(\frac{h}{2}+c\right) + \frac{1}{24}g'(c+h) + R(g(th+c))\right]$$

$$= -\frac{h}{24}g'(c) + hg\left(\frac{h}{2}+c\right) + \frac{h}{24}g'(c+h) + hR(g(th+c))$$

$$R(g(th+c)) = -\frac{7}{5760}h^5 g^{(4)}(\xi)$$

$$\int_a^b g(x)dx = \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} g(x)dx$$

$$\sum_{k=0}^{n-1} \left[-\frac{h}{24} g'(x_k) + hg\left(x_k + \frac{h}{2}\right) + \frac{h}{24} g'(x_k + h) \right] - \sum_{k=0}^{n-1} \frac{7}{5760} h^5 g^{(4)}(\xi_k)$$

$$= h \left[-\frac{1}{24} g'(a) + \sum_{k=0}^{h-1} g\left(a + \left(k + \frac{1}{2}\right) h\right) + \frac{1}{24} g'(b) \right] - \frac{7(b-a)^5}{5760 n^4} g^(4)(\xi);$$

■

Problem 40 (Gautschi, Ch.3, 52, pag.203) *Consider a quadrature rule of the form*

$$\int_0^1 x^\alpha f(x)dx \approx Af(0) + B \int_0^1 f(x)dx, \quad \alpha > -1, \alpha \neq 0$$

(a) Determine A and B such that the formula has degree of exactness $d = 1$.

(b) Let $R(f)$ be the error functional of the rule determined in (a). Show that the Peano kernel $K_1(t) = R_{(x)}((x-t)_+)$ is positive definite if $\alpha > 0$ and negative definite if $\alpha < 0$.

(c) Based on the result of (b), determine the constant e_2 in $R(f)_1 = e_2 f''(\xi)$, $0 < \xi < 1$.

Solution. (a) $\displaystyle\int_0^1 x^\alpha dx = \frac{1}{\alpha+1} = A + B$

$$\int_0^1 x^\alpha x dx = \frac{1}{\alpha+2} = A \cdot 0 + \frac{B}{2}$$

$$A = \frac{\alpha}{(\alpha+1)(\alpha+2)}, \quad B = \frac{2}{\alpha+2}$$

(b) $\displaystyle R(f) = \int_0^1 K(t) f''(t)dt$

$$K(t) = \int_0^1 x^\alpha (x-t)_+ dx - \frac{\alpha}{(\alpha+1)(\alpha+2)}(-t)_+ - \frac{2}{\alpha+2} \int_0^1 (x-t)_+ dt$$

$$= \int_0^1 x^\alpha (x-t)_+ dx - \frac{2}{\alpha+2} \cdot \frac{(1-t)^2}{2}$$

$$\int_t^1 x^\alpha(x-t)dx - \frac{1}{\alpha+2}(1-t)^2 = \frac{x^{\alpha+2}}{\alpha+2}\Big|_t^1 - \frac{tx^{\alpha+1}}{\alpha+1}\Big|_t^1 - \frac{1}{\alpha+2}(1-t)^2$$

$$= \frac{1-t^{\alpha+2}}{\alpha+2} - t\frac{1-t^{\alpha+1}}{\alpha+1} - \frac{1}{\alpha+2}(1-t)^2$$

$$= \frac{-t^{\alpha+2}+(\alpha+2)t-\alpha-1}{(\alpha+1)(\alpha+2)} = \frac{t^{\alpha+2}-(\alpha+2)t+(\alpha+1)}{(\alpha+1)(\alpha+2)}$$

$$t_{1,2} = \frac{\alpha+2 \pm \sqrt{(\alpha+2)^2-\alpha-1}}{2} = \frac{t^{\alpha+2}+(\alpha+1)(1-t)-t}{(\alpha+1)(\alpha+2)}$$

$$const(b) = \frac{t(t^{\alpha+1}-1)+(\alpha+1)(1-t)}{(\alpha+1)(\alpha+2)}$$

(c) $R(f) = \dfrac{1}{2!}f''(\xi)R(e_2) = \dfrac{\alpha}{6(\alpha+3)(\alpha+2)}f''(\xi)$ ■

Problem 41 (Gautschi, Ch.3, 55, pag.204) *Let*

$$a = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_4 = b, \quad x_k = a+kh, \quad h = \frac{b-a}{n}$$

be a subdivision of $[a,b]$ *into* n *equal subintervals.*

(a) Derive an elementary quadrature formula for the integral $\displaystyle\int_{x_k}^{x_{k+1}} f(x)dx$ *including a remainder term, by approximating* f *by the cubic Hermite interpolation polynomial* $(H_3f)(x; x_k, x_k, x_{k+1}, x_{k+1})$ *and then integrating over* $[x_k, x_{k+1}]$. *Interpret the result.*

(b) Develop the formula obtained in (a) into a composite quadrature rule, with remainder term, for the integral $\displaystyle\int_a^b f(x)dx$.

Solution. (a) The Hermite interpolation polynomial is

$$(H_3f)(x; x_k, x_k, x_{k+1}, x_{k+1}) = h_{00}(x)f(a)$$

$$+h_{01}(x)f'(a) + h_{10}(x)f(b) + h_{11}(x)f'(b)$$

where

$$h_{00}(x) = \frac{(x-x_{k+1})^2}{(x_k-x_{k+1})^3}(3x_k - x_{k+1} - 2x)$$

$$h_{01}(x) = \frac{x-x_k}{(x_k-x_{k+1})^2}(x-x_{k+1})^2$$

$$h_{10}(x) = \frac{(x-x_k)^2}{(x_{k+1}-x_k)^3}(3x_{k+1}-x_k-2x)$$

$$h_{11}(x) = (x-x_{k+1})\frac{(x-x_k)^2}{(x_{k+1}-x_k)^2}$$

$$(R_3 f)(x) = \frac{(x-x_k)^2(x-x_{k+1})^2}{4!}f^{(4)}(\xi)$$

Integrating term by term one obtains

$$\int_a^b f(x)dx = \frac{x_{k+1}-x_k}{2}[f(x_k)+f(x_{k+1})]$$

$$+\frac{(x_{k+1}-x_k)^2}{12}[f'(x_k)-f'(x_{k+1})] - \frac{(x_{k+1}-x_k)^5}{720}f^{(4)}(\xi)$$

(b) $\displaystyle\int_a^b f(x)dx = \sum_{k=0}^{n-1}\int_{x_k}^{x_{k+1}} f(x)dx$

$$= \sum_{k=0}^{n-1}\left\{\frac{h}{2}[f(x_k)+f(x_{k+1})] + \frac{h^2}{12}[f'(x_k)-f'(x_{k+1})] - \frac{h^5}{720}f^{(4)}(\xi_k)\right\}$$

$$= \frac{h}{2}\left[f(a) + 2\sum_{k=1}^{n-1} f(x_k) + f(b)\right]$$

$$+\frac{h^2}{12}[f'(a)-f'(b)] - \frac{(b-a)^5}{720n^4}f^{(4)}(\xi)$$

■

Problem 42 *(Gautschi, Ch.3, 56, pag.204)*

(a) Given a function $g(x,y)$ on the unit square $0 \le x \le 1$, $0 \le y \le 1$, determine a bilinear polynomial $p(x,y) = a + bx + cy + dxy$ such that p has the same value as g on the four corners of the square.

(b) Use (a) to obtain a cubature formula for $\int_0^1 \int_0^1 g(x,y)dxdy$ that involves the values of g at the fours corners of the unit square. What rule does this reduce to if g is a function of x only (i.e. does not depend on y)?

(c) Use (b) to find a "composite cubature rule" for $\int_0^1 \int_0^1 g(x,y)dxdy$ involving the values $g_{i,j} = g(ih, jh)$, $i, j = 0, 1, \ldots, n$, where $h = 1/n$.

Solution. (a) $g(x,y) = (1-x)(1-y)g(0,0) + (1-x)yg(0,1) + x(1-y)g(1,0) + xyg(1,1)$

$$+\frac{x(x-1)}{2}\frac{\partial^2}{\partial x^2}g(\xi,y) + \frac{y(y-1)}{2}\frac{\partial^2}{\partial y^2}g(x,\eta_1)$$

$$-\frac{x(x-1)y(y-1)}{4}\frac{\partial^4}{\partial x^2 \partial y^2}f(\xi_2,\eta_2)$$

$$p(x,y) = (1-x-y+xy)g_{00} + (y-xy)g_{01} + (x-xy)g_{10} + xyg_{11}$$

$$= g_{00} + (g_{10}-g_{00})x + (g_{01}-g_{00})y + (g_{11}-g_{10}-g_{01}+g_{00})xy$$

(b) $\displaystyle\int_0^1\int_0^1 g(x,y)dxy = \int_0^1\int_0^1 p(x,y) + R_{11}(g)$

$$\int_0^1\int_0^1 p(x,y)dxdy = \frac{1}{4}[g_{00}+g_{01}+g_{10}+g_{11}]$$

$$R_{11}(g) = -\frac{1}{12}g^{(2,0)}(\xi_1,\eta_1) - \frac{1}{12}g^{(0,2)}(\xi_2,\eta_2) - \frac{1}{144}g^{2,2}(\xi_3,\eta_3)$$

(c) $\displaystyle\int_0^1\int_0^1 g(x,y)dxdy \approx \sum_{j=0}^{n-1}\sum_{j=0}^{n-1}\frac{1}{4}[g_{i+1,j+1}+g_{i,j+1}+g_{i+1,j}+g_{ij}]$

$$= \frac{1}{4}\left[g_{00}+g_{0n}+g_{n0}+g_{nn}+2\sum_{i=1}^{n-1}(g_{i0}+g_{in})\right.$$

$$\left.+2\sum_{j=}^{n-1}(g_{0j}+g_{nj}) + 4\sum_{i=1}^{n-1}\sum_{j=1}^{n-1}g_{ij}\right]$$

■

Problem 43 *(a) Use the central difference quotient approximation* $f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}$ *of the first derivative to obtain an approximation of* $\frac{\partial^2 u}{\partial x \partial y}(x,y)$ *for a function* u *of two variables.*

(b) Use Taylor expansion of a function of two variables to show that the error of the approximation derived in (a) is $O(h^2)$*.*

Solution.

(a) We have

$$\begin{aligned}
\frac{\partial^2 f}{\partial x \partial y} &= \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) \\
&\approx \frac{\partial}{\partial y}\left(\frac{f(x+h,y)+f(x-h,y)}{\partial x}\right) \\
&\approx \frac{1}{2h}\left[\frac{f(x+h,y+h)-f(x+h,y-h)}{2h} - \frac{f(x-h,y+h)-f(x-h,y-h)}{2h}\right] \\
&\approx \frac{1}{4h^2}\left[f(x+h,y+h)-f(x+h,y-h)-f(x-h,y+h)+f(x-h,y-h)\right]
\end{aligned}$$

(b) Since the approximation obtained in (a) is an even function of h, its Taylor expansion involves only even powers of h. The constant term in

$$\frac{1}{2}h^2\left[(u_{xx}+2u_{xy}+u_{yy})-(u_{xx}-2u_{xy}+u_{yy})-(u_{xx}-2u_{xy}+u_{yy})\right.$$
$$\left.+(u_{xx}+2u_{xy}+u_{yy})\right]+O(h^4)=\frac{1}{2}h^2[8u_{xy}]+O(h^4)=4h^2u_{xy}+O(h^4),$$

where all partial derivatives are evaluated at (x, y). Thus, dividing by $4h^2$, we see that the approximation equals the exact value u_{xy} plus a term of $O(h^2)$.

■

Problem 44 *Consider the integral $I = \int_{-1}^{1} |x| \, \mathrm{d}\, x$, whose exact value is evidently 1. Suppose I is approximated (as it stands) by the composite trapezoidal rule $T(h)$ with $h = 2/n$, $n = 1, 2, 3, \ldots$*

(a) Show (without any computation) that $T(2/n) = 1$ if n is even.

(b) Determine $T(2/n)$ for n odd and comment on the speed of convergence.

Solution.

(a) If n is even, then $T(2/n)$ is the trapezoidal rule applied to $[-1, 0]$ plus the trapezoidal rule applied to $[0, 1]$, each being exact.

(b) Denoting by $T(h)[a,b]$ the composite trapezoidal rule applied to $[a,b]$ with steplength h, we have, when n is odd,

$$\begin{aligned} T(2/n)[-1,1] &= T(2/n)[-1,-1/n] + T(2/n)[1/n,1] + \frac{2}{n}\left[\frac{1}{2}\frac{1}{n} + \frac{1}{2}\frac{1}{n}\right] \\ &= \int_{-1}^{-1/n} |x|\,\mathrm{d}\,x + \int_{1/n}^{1} |x|\,\mathrm{d}\,x + \frac{2}{n}\frac{1}{n} \\ &= 2\int_{1/n}^{1} x\mathrm{d}\,x + \frac{2}{n^2} = 2\left[\frac{x^2}{2}\right]_{1/n}^{1} + \frac{2}{n^2} \\ &= 1 - \frac{1}{n^2} + \frac{2}{n^2} = 1 + \frac{1}{n^2}. \end{aligned}$$

Thus, we still have the usual $O(h^2)$ convergence, even though the integrand is only in $C[-1,1]$.

■

Problem 45 *Consider a quadrature formula of the form*

$$\int_0^1 f(x)\mathrm{d}\,x \approx a_0 f(0) + a_1 f'(0) + \sum_{k=1}^{n} w_k f(x_k) + b_0 f(1).$$

(a) *Call the formula "Hermite-interpolatory" if the right-hand side is obtained by integrating on the left instead of f the (Hermite) interpolation polynomial p satisfying*

$$\begin{aligned} p(0) = f(0),\ p'(0) = f'(0),\ p(1) = f(1) \\ p(x_k) = f(x_k), \quad k = 1, 2, \ldots, n. \end{aligned}$$

What degree of exactness does the formula have in this case (regardless of how the nodes xk are chosen, as long as they are mutually distinct and strictly inside the interval $[0,1]$)?

(b) *What is the maximum degree of exactness expected to be if all coefficients and nodes x_k are allowed to be freely chosen?*

(c) *Show that for the maximum degree of exactness to be achieved, it is necessary that $\{x_k\}$ are the zeros of the polynomial π_n of degree n which is orthogonal on $[0,1]$ with respect to the weight function $w(x) = x^2(1-x)$. Identify this polynomial in terms of one of the classical orthogonal polynomials.*

(d) *Show that the choice of the x_k in (c) together with the requirement of the quadrature formula to be Hermite-interpolatory is sufficient for the maximum degree of exactness to be attained.*

Solution. ∎

Problem 46 *Show that the Gauss–Radau as well as the Gauss–Lobatto formulae are positive if the weight function w is nonnegative and not identically zero. (Hint: modify the proof given for the Gauss formula.) What are the implications with regard to convergence as $n \to \infty$ of the formulae?*

Solution. For the Gauss–Radau formula with $t_1 = a$,

$$\int_a^b w(t)f(t)\mathrm{d}\,t = w_1 f(a) + \sum_{k=2}^{n} w_k f(x_k) + R_n(f)$$
$$R_n(\mathbb{P}_{2n-2}) = 0,\ n \geq 2,$$

let

$$p_1(t) = \prod_{k=2}^{n} \left(\frac{t - t_k}{a - t_k}\right)^2$$
$$p_j(t) = \frac{t-a}{t_j - a} \prod_{\substack{k=2 \\ k \neq j}}^{n} \left(\frac{t - t_k}{t_j - t_k}\right)^2,\ j = 2, \ldots, n.$$

Here, $p_1 \in \mathbb{P}_{2n-2}$ and $p_j \in \mathbb{P}_{2n-3}$ for $j = 2, \ldots, n$, and $p_1 \geq 0$, $p_j \geq 0$ on $[a, b]$. Applying the Gauss–Radau formula to $f = p_1$ and $f = p_j$ then gives

$$0 < w_1 = \int_a^b w(t)p_1(t)\mathrm{d}\,t = w_1$$
$$0 < w_j = \int_a^b w(t)p_1(t)\mathrm{d}\,t = w_j, \quad j = 2, \ldots, n.$$

The reasoning is the same for the Gauss–Radau formula with $t_n = b$.

For the Gauss–Lobatto formula

$$\int_a^b w(t)f(t)\mathrm{d}\,t = w_1 f(a) + \sum_{k=2}^{n-1} w_k f(x_k) + w_n f(b) + R_n(f)$$
$$R_n(\mathbb{P}_{2n-3}) = 0,\ n \geq 3,$$

one argues similarly, taking

$$p_1(t) = \frac{b-t}{b-a}\prod_{k=2}^{n-1}\left(\frac{t-t_k}{a-t_k}\right)^2$$

$$p_j(t) = \frac{t-a}{t_j-a}\frac{b-t}{b-t_j}\prod_{k=2}^{n-1}\left(\frac{t-t_k}{a-t_k}\right)^2,\ j=2,\dots,n-1$$

$$p_n(t) = \frac{t-a}{b-a}\prod_{k=2}^{n-1}\left(\frac{t-t_k}{b-t_k}\right)^2$$

Since both formulae have degrees of exactness that tend to infinity as $n \to \infty$, their convergence is proved in the same way as for Gaussian quadrature rules. ∎

Problem 47 *Let $\pi_n(.,w)$ be the nth-degree orthogonal polynomial with respect to the weight function w on $[a,b]$, t_1, t_2, …, t_n its n zeros, and w_1, w_2, …, w_n the n Gauss weights.*

(a) Assuming $n > 1$, show that the n polynomials π_0, π_1, …, π_{n-1} are also orthogonal with respect to the discrete inner product $(u,v) = \sum_{\nu=1}^n w_\nu u(t_\nu)v(t_\nu)$.

(b) With $\ell_i(t) = \prod_{k\neq i}\frac{t-t_k}{t_i-t_k}$, $i = 1,2,\dots,n$, denoting the elementary Lagrange interpolation polynomials associated with the nodes t_1, t_2, …, t_n, show that

$$\int_a^b \ell_i(t)\ell_k(t)w(t)\mathrm{d}\,t = 0.$$

Solution.

(a) Use the Gauss quadrature rule and the fact that $\pi_k\pi_\ell \in \mathbb{P}_{2n-2}$ for $k,\ell = 0,1,\dots,n-1$, to obtain

$$0 = \int_a^b \pi_k(t)\pi_\ell(t)w(t)\mathrm{d}\,t = \sum_{\nu=1}^n \pi_k(t_\nu)\pi_\ell(t_\nu)w(t_\nu),\ k\neq\ell.$$

(b) Apply Gaussian quadrature: since $\ell_i\ell_k \in \mathbb{P}_{2n-2}$, we get

$$\begin{aligned}\int_a^b \ell_i(t)\ell_k(t)w(t)\mathrm{d}\,t &= \sum_{\nu=1}^n \ell_i(t_\nu)\ell_k(t_\nu)w(t_\nu)\\ &= \sum_{\nu=1}^n w_\nu\delta_{i\nu}\delta_{k\nu} = 0,\ i\neq k.\end{aligned}$$

■

Problem 48 *Consider the Hermite interpolation problem: Find* $p \in P_{2n-1}$ *such that*

$$p(\tau_\nu) = f(\tau_\nu), \; p'(\tau_\nu) = f'(\tau_\nu), \; \nu = 1, 2, \ldots, n. \qquad ((*))$$

There are "elementary Hermite interpolation polynomials" h_ν, k_ν *such that the solution of (*) can be expressed (in analogy to Lagrange's formula) in the form*

$$p(t) = \sum_{\nu=1}^{n} \left[h_\nu(t) f_\nu + k_\nu(t) f'_\nu \right].$$

(a) Seek h and k in the form

$$h_\nu(t) = (a_\nu + b_\nu t)\, \ell_\nu^2(t), \; k_\nu(t) = (c_\nu + d_\nu t)\, \ell_\nu^2(t),$$

where ℓ_ν *are the elementary Lagrange polynomials. Determine the constants* a_ν, b_ν, c_ν, d_ν.

(b) Obtain the quadrature rule

$$\int_a^b f(t) w(t) \mathrm{d}\, t = \sum_{\nu=1}^{n} \left[\lambda_\nu f(\tau_\nu) + \mu_\nu f'(\tau_\nu) \right] + R_n(f)$$

with the property that $R_n(f) = 0$ *for all* $f \in \mathbb{P}_{2n-1}$.

(c) What conditions on the node polynomial $\omega_n(t) = \prod_{\nu=1}^{n} (t - t_\nu)$ *(or on the nodes* τ_ν*) must be imposed in order that* $\mu_\nu = 0$ *for* $\nu = 1, 2, \ldots, n$*?*

Solution.

(a) We must have

$$h_\nu(\tau_\nu) = 1, \; h_\nu(\tau_\nu) = 0,$$

the other required equations $h_\nu(\tau_\mu) = h'_\nu(\tau_\mu) = 0$, $\mu \neq \nu$, being automatically satisfied in view of the proposed form of h_ν. Thus,

$$a_\nu + b_\nu \tau_\nu = 1, \; b_\nu + (a_\nu + b_\nu \tau_\nu) \cdot 2\ell_\nu(\tau_\nu)\, \ell'_\nu(\tau_\nu) = 0,$$

that is,

$$\begin{aligned} a_\nu + b_\nu \tau_\nu &= 1, \\ b_\nu + 2\ell'_\nu(\tau_\nu) &= 0. \end{aligned}$$

Solving this for a_ν and b_ν and inserting the result in the proposed form of h_ν gives

$$h_\nu(t) = \left[1 - 2(t-\tau_\nu)\ell'_\nu(\tau_\nu)\right] \ell^2_\nu(t), \quad \nu = 1,2,\ldots,n.$$

Likewise, k_ν must satisfy

$$k_\nu\,(\tau_\nu) = 0,\ k'_\nu\,(\tau_\nu) = 1$$

giving

$$c_\nu + d_\nu\tau_\nu = 0,\ d_\nu + (c_\nu + d_\nu\tau_\nu)\cdot 2\ell_\nu(\tau_\nu)\ell'_\nu(\tau_\nu) = 1,$$

that is,

$$c_\nu + d_\nu\tau_\nu = 0, \quad d_\nu = 1.$$

Thus, $c_\nu = -\tau_\nu$, and

$$k_\nu(t) = (t-\tau_\nu)\ell^2_\nu(t), \quad \nu = 1,2,\ldots,n.$$

Note that

$$\ell'_\nu(\tau_\nu) = \sum_{\mu\neq\nu} \frac{1}{\tau_\nu - \tau_\mu}.$$

(b) The quadrature rule in question is

$$\int_a^b f(t)w(t)\mathrm{d}\,t = \int_a^b p(t)w(t)\mathrm{d}\,t + R_n(f),$$

which clearly has degree of exactness $2n-1$. Using (a), we get

$$\begin{aligned}\int_a^b p(t)w(t)\mathrm{d}\,t &= \int_a^b \sum_{\nu=1}^n \left[h_\nu(t)f_\nu + k_\nu\,(t)\,f'_\nu\right] w(t)\mathrm{d}\,t \\ &= \sum_{\nu=1}^n \left[f_\nu \int_a^b h_\nu(t)w(t)\mathrm{d}\,t + f'_\nu \int_a^b k_\nu\,(t)\,w(t)\mathrm{d}\,t\right].\end{aligned}$$

Thus

$$\lambda_\nu = \int_a^b h_\nu(t)w(t)\mathrm{d}\,t, \quad \mu_\nu = \int_a^b k_\nu\,(t)\,w(t)\mathrm{d}\,t, \quad \nu = 1,2,\ldots,n.$$

(b) For all μ to be zero, we must have

$$\int_a^b k_\nu(t)\, w(t) \mathrm{d}\, t = 0, \quad \nu = 1, 2, \dots, n.$$

or, by the results in (a), noting that $\ell_\nu(t) = \frac{\omega_n(t)}{(t-\tau_\nu)\omega_n'(\tau_\nu)}$,

$$\frac{1}{\omega_n'(\tau_\nu)} \int_a^b \frac{\omega_n(t)}{(t-\tau_\nu)\omega_n'(\tau_\nu)} \omega_n(t) w(t) \mathrm{d}\, t = 0, \quad \nu = 1, 2, \dots, n.$$

that is,

$$\int_a^b \ell_\nu(t) \omega_n(t) w(t) \mathrm{d}\, t = 0, \quad \nu = 1, 2, \dots, n.$$

Since $\{\ell_\nu(t)\}_{\nu=1}^n$ forms a basis of $\mathbb{P}_{n-1}$ (the ℓ_ν are linearly independent and span $\mathbb{P}_{n-1}$), ω_n must be orthogonal with respect to the weight function w to all polynomials of lower degree, i.e., $\omega_n(t) = \pi_n(t; w)$. We get the Gauss quadrature rule.

■

Problem 49 *(a) Use the method of undetermined coefficients to obtain an integration rule (having degree of exactness $d = 2$) of the form*

$$\int_0^1 y(s) \mathrm{d}\, s \approx a y(0) + b y(1) - c\left[y'(1) - y'(0)\right] + R(f).$$

(b) Transform the rule in (a) into one appropriate for approximating $\int_x^{h+x} f(t) \mathrm{d}\, t$.

(c) Obtain a composite integration rule based on the formula in (b) for approximating $\int_a^b f(t) \mathrm{d}\, t$. Interpret the result.

Solution.

(a) Putting in turn $y(s) = 1$, $y(s) = s$, $y(s) = s^2$, one gets

$$\begin{aligned} a + b + 0c &= 1 \\ 0a + b - 0c &= \frac{1}{2} \\ 0a + b - 2c &= \frac{1}{3} \end{aligned}$$

Solution is: $\left[a = \frac{1}{2}, b = \frac{1}{2}, c = \frac{1}{12}\right]$, that is,

$$\int_0^1 y(s) \mathrm{d}\, s = \frac{1}{2}\left[y(0) + y(1)\right] - \frac{1}{12}\left[y'(1) - y'(0)\right] + R(f)$$

(b) The transformation $t = x + hs$, $dt = hds$ yields

$$\int_x^{x+h} f(t)\mathrm{d}\,t = h\int_0^1 (x+hs)\,\mathrm{d}\,s \approx \frac{h}{2}\left[f(x)+f(x+h)\right] - \frac{h^2}{12}\left[f'(x+h)-f'(h)\right]$$

(c) Letting $h = (b-a)/n$, $x_k = a + kh$, $f_k = f(x_k)$, $f'_k = f'(x_k)$, $k = 0, 1, \ldots, n$, one finds, using (b), that

$$\begin{aligned}\int_a^b f(t)\mathrm{d}\,t &= \sum_{k=0}^{n-1}\int_{x_k}^{x_k+h} f(t)\mathrm{d}\,t \approx \frac{h}{2}\left[(f_0+f_1)+(f_1+f_2)+\cdots\right.\\ &\left.+\ (f_{n-1}+f_n)\right] - \frac{h^2}{12}\left[\left(f'_1-f'_0\right)+\left(f'_2-f'_{10}\right)+\cdots+\left(f'_n-f'_{n-1}\right)\right]\\ &= h\left(\frac{1}{2}f_0+f_1+\cdots+f_{n-1}+\frac{1}{2}f_n\right) - \frac{h^2}{12}\left[f'(b)-f'(a)\right].\end{aligned}$$

This may be interpreted as a composite trapezoidal rule with "end correction". The correction approximates the error term of the composite trapezoidal rule:

$$-\frac{b-a}{12}h^2 f''(\xi) \approx -\frac{h^2}{12}\left[f'(b)-f'(a)\right].$$

■

Chapter 4

Nonlinear Equation

Problem 50 *(Choosing the starting value for Newton's method). If $f(a)f(b) < 0$ and $f'(x)$ and $f''(x)$ are nonzero and preserve signs over $[a, b]$, then proceeding from the initial approximation $x_0 \in [a, b]$ s.t.*

$$f(x_0)f''(x_0) > 0 \tag{4.1}$$

it is possible, by using Newton's method to compute the sole root ξ of $f(x) = 0$ to any degree of accuracy. $f \in C^2[a, b]$.

Proof. For example, suppose $f(a) > 0$, $f(b) < 0$, $f'(x) > 0$, $f''(x) > 0$ for $x \in [a, b]$ (the other cases are considered similarly).

By inequality (4.1) we have $f(x_0) > 0$ (we can, say, take $x_0 = b$). By mathematical induction we prove that all approximation $x_n > \xi$ $(n \in \mathbb{N})$ and hence $f(x_n) > 0$. Indeed, first of all $x_0 > \xi$. Now let $x_n > \xi$. Put

$$\xi = x_n + (\xi - x_n).$$

Using Taylor's formula, we get

$$0 = f(\xi) = f(x_n) + f'(x_n)(\xi - x_n) + \frac{1}{2}f''(c_n)(\xi - x_n)^2$$

where $\xi < c_n < x_n$.

Since $f''(x) > 0$ we have

$$f(x_n) + f'(x_n)(\xi - x_n) < 0$$

and hence

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} > \xi$$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{4.2}$$

Taking into consideration the sign of $f(x_n)$ and $f'(x_n)$ we have from formula of Newton's method (4.2) $x_{n+1} < x_n$, that is the sequence (x_n) is a bounded and decreasing sequence. Therefore, the limit $\overline{\xi} = \lim\limits_{n\to\infty}$ exists.

Passing to the limit in (3) we have

$$\overline{\xi} = \overline{\xi} - \frac{f(\overline{\xi})}{f'(\xi)}$$

or $f(\overline{\xi}) = 0$, whence $\overline{\xi} = \xi$, and the proof is complete. ■

Problem 51 *If*

(1) $f \in C(\mathbb{R})$,

(2) $f(a)f(b) < 0$,

(3) $f'(x) \neq 0$ *for* $x \in [a, b]$

(4) $f''(x)$ *exists and preserves sign, then any value* $c \in [a, b]$ *may be taken for the initial approximation* x_0 *when using Newton's method to find a root of the equation* $f(x) = 0$ *lying in* (a, b). *One can for instance, take* $x_0 = a$ *or* $x_0 = b$.

Proof. Suppose say, $f'(x) > 0$, $f''(x) > 0$, $x_0 = c$, $c \in [a, b]$. If $f(c) = 0$, then $\xi = c$ is a root and the problem is solved. If $f(c) > 0$ then the foregoing reasoning holds true and the Newton process with initial value c converges to the root $\xi \in (a, b)$.

Finally, if $f(c) < 0$, then we find the value

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = c - \frac{f(c)}{f'(c)} > c.$$

Using Taylor's formula we have

$$f(x_1) = f(c) - \frac{f(c)}{f'(c)} f'(c) + \frac{1}{2}\left[\frac{f(c)}{f'(c)}\right]^2 f''(\overline{c}) = \frac{1}{2}\left[\frac{f(c)}{f'(c)}\right]^2 f''(\overline{c}) > 0,$$

where $\overline{c} \in (c, x_1)$.

Thus

$$f(x_1)f''(x_1) > 0.$$

Besides, from the condition $f''(x) > 0$ it follows that f' is an increasing function and hence $f'(x) > f'(a) > 0$ for $x > a$. It is thus possible to take x_1 for the initial value of the Newton process converging to some root $\overline{\xi}$ of the function. ■

Problem 52 *(21 Gautschi, Ch.4, pag.253)*

(a) Show that Newton's iteration

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right), \quad a > 0$$

for computing the square root $\alpha = \sqrt{a}$ satisfies

$$\frac{x_{n+1} - \alpha}{(x_n - \alpha)^2} = \frac{1}{2x_n}$$

Hence, directly obtain the asymptotic error constant.

(b) What is the analogous formula for the cube root.

Solution. $x_{n+1} - \alpha = (x_n - \alpha)^2 \frac{f[x_n, x_n, \alpha]}{f[x_n, x_n]} = (x_n - \alpha)^2 \frac{f''(\xi)}{2f'(x_n)} = (x_n - \alpha)^2 \frac{1}{2x_n}$, so ass.err. constant is

$$\lim_{n\to\infty} \frac{x_{n+1} - \alpha}{(x_n - \alpha)^2} = \lim_{n\to\infty} \frac{1}{2x_n} = \frac{1}{2\sqrt{a}}$$

(b) $f(x) = x^3 - a = 0$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^3 - a}{3x_n^2} = \frac{3x_n^3 - x_n^3 + a}{3x_n^2}$$

$$= \frac{2x_n^3 + a}{3x_n^2} = \frac{1}{3}\left(2x_n + \frac{a}{x_n^2}\right)$$

■

Problem 53 *(Gautschi, Ch.4, 22, pag.253)*

Consider Newton's method

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right), \quad a > 0$$

for computing the square root $\alpha = \sqrt{a}$. Let $d_n = x_{n+1} - x_n$.

(a) Show that

$$x_n = \frac{a}{d_n + \sqrt{d_n^2 + a}}$$

(b) Use (a) to show that

$$|d_{n+1}| = \frac{d_n^2}{2\sqrt{d_n^2 + a}}, \quad n \in \mathbb{N}.$$

Discuss the significance of this result with regard to the overall behavior of Newton's iteration in this case.

(c) Show that for this method, the number of correct digits is roughly doubles at each step.

(Hint. Put $x_n = \sqrt{a}(1+\delta)$ and compute x_{n+1}).

Solution. (a) $d_n = x_{n+1} - x_n =$

$$\frac{1}{2}\left(x_n + \frac{a}{x_n}\right) - x_n = \frac{1}{2}\left(-x_n + \frac{a}{x_n}\right) \Rightarrow$$

$$x_n^2 + 2d_n x_n - a = 0 \Rightarrow x_n^{(1,2)} = -d_n \pm \sqrt{d_n^2 + a}$$

only $x_n = -d_n + \sqrt{d_n^2 + a}$ is convenient

$$x_n = \frac{d_n^2 - (d_n^2 + a)}{-d_n - \sqrt{d_n^2 + a}} = \frac{a}{d_n + \sqrt{d_n^2 + a}}$$

(b) $x_{n+1} - x_n = d_n = -d_{n+1} + \sqrt{d_{n+1}^2 + a} + d_n - \sqrt{d_n^2 + a} \Rightarrow$

$$-\underbrace{d_{n+1}}_{y} + \sqrt{d_{n+1}^2 + a} = \underbrace{\sqrt{d_n^2 + a}}_{b}$$

$$\sqrt{y^2 + a} = b + y \Rightarrow y^2 + a = b^2 + 2by + y^2$$

$$y = \frac{a - b^2}{2b} \Rightarrow |d_{n+1}| = \frac{d_n^2}{2\sqrt{d_n^2 + a}}, \quad n \in \mathbb{N}$$

$$\frac{|d_{n+1}|}{|d_n|^2} = \frac{1}{2\sqrt{d_{n-1}^2 + a}} \to \frac{1}{2\sqrt{a}} \text{ since } d_n \to 0$$

(c) $x_n = \sqrt{a}(1+\delta)$, δ - relative error

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right) = \frac{1}{2}\left(\sqrt{a}(1+\delta) + \frac{a}{\sqrt{a}(1+\delta)}\right)$$

$$= \frac{\sqrt{a}}{2}(1 + \delta + (1 - \delta + \delta^2 + \dots)) \approx \sqrt{a}\left(1 + \frac{\delta^2}{2}\right)$$

■

Problem 54 (Gautschi, Ch.4, 19, pag.252) *(a) Derive an iterative scheme, using only addition and multiplication, for computing the reciprocal $\frac{1}{a}$ of some positive number a.*

(b) *For what starting values* x_0 *does the algorithm in (a) converge? What happens if* $x_0 < 0$*?*

(c) *Since in (binary) floating point-arithmetic it suffices to find the reciprocal of the mantissa, assume* $1 \le a < 2$*, or by increasing the exponent with one unit* $\frac{1}{2} \le a < 1$*. Show that in this last case*

$$\left| x_{n+1} - \frac{1}{a} \right| < \left| x_n - \frac{1}{a} \right|^2 .$$

(d) *Using the result of (c), estimate how many iterations are required, at most, to obtain* $\frac{1}{a}$ *with an error less than* 2^{-48}*, if one takes* $x_0 = \frac{3}{2}$*.*

Solution. (a) $f(x) = a - \frac{1}{x}$, $f'(x) = \frac{1}{x^2}$

$$x_{n+1} = x_n - \frac{f(x)}{f'(x)} = x_n - \frac{a - \frac{1}{x_n}}{\frac{1}{x_n^2}} = x_n(2 - a x_n)$$

Stopping criterion $|x_{n+1} - x_n| < \varepsilon$

(b) (1) $\frac{1}{a} - x_n = \frac{1}{a} - 2x_{n-1} + a x_{n-1}^2$

$$= a \left(\frac{1}{a} - x_{n-1} \right)^2 = \cdots = a^{2^n - 1} \left(\frac{1}{a} - x_0 \right)^{2n} = \frac{1}{a}(1 - a x_0)^{2n}$$

(x_n) convergent $\Leftrightarrow |1 - a x_0| < 1 \Leftrightarrow 0 < a x_0 < 2$

For $x_0 < 0$, (x_n) diverges.

(c) For $\frac{1}{2} \le a < 1$, (1) $\Rightarrow$

$$\left| x_{n+1} - \frac{1}{a} \right| < \left| x_n - \frac{1}{a} \right|^2, \quad n \in \mathbb{N}$$

(d) $\left| x_{n+1} - \frac{1}{a} \right| < \left| x_n - \frac{1}{a} \right|^2 < \cdots < \left| x_0 - \frac{1}{a} \right|^{2^{n+1}}$

$$= \left| \frac{3}{2} - \frac{1}{a} \right|^{2^{n+1}} < \left(\frac{1}{2} \right)^{2^{n+1}} = \frac{1}{2^{2^{n+1}}} \Rightarrow 2^{n+1} \ge 48 \text{ (or 53)}$$

$$n = 5!$$

■

Problem 55 (Gautschi, Ch.4, 18, pag.252) *Consider "Kepler's equation"*

$$f(x) = 0, \quad f(x) = x - \varepsilon \sin x - \eta, \quad 0 < |\varepsilon| < 1, \ \eta \in \mathbb{R}$$

where ε, η are parameters.

(a) Show that for each ε, η there is exact one real root $\alpha = \alpha(\varepsilon, \eta)$. Furthermore

$$\eta - |\varepsilon| \leq \alpha(\varepsilon, \eta) \leq \eta + \varepsilon.$$

(b) Writing the equation in fixed point form

$$x = \varphi(x), \quad \varphi(x) = \varepsilon \sin x + \eta$$

show that the fixed point iteration $x_{n+1} = \varphi(x_n)$ converges for arbitrary starting value x_0.

(c) Let m be an integer such that $m\pi < \eta < (m+1)\pi$. Show that Newton's method with starting value

$$x_0 = \begin{cases} (m+1)\pi, & \text{if } (-1)^m \varepsilon > 0; \\ m\pi, & \text{otherwise.} \end{cases}$$

is guaranteed to converge (monotonically) to $\alpha(\varepsilon, \eta)$.

(d) Estimate the asymptotic constant c of Newton's method.

Solution. (a) $f(\eta - |\varepsilon|) = \eta - |\varepsilon| - \varepsilon \sin(\eta - \varepsilon) - \eta < 0$

$$f(\eta + |\varepsilon|) = \eta + |\varepsilon| - \varepsilon \sin(\eta + |\varepsilon|) - \eta > 0$$

(b) $|\varphi'(x)| = |-\varepsilon \cos x| \leq |\varepsilon| < 1$

(c) On the interval $(m\pi, (m+1)\pi)$, $f(x)$ preserves its convexity or concavity since $f''(x) = \varepsilon \sin x$.

$$f'(x) = 1 - \varepsilon \cos x > 0$$

convexity right endpoint $f(x_1)f''(x_1) > 0$
concavity left endpoint

(d) $c = \dfrac{f''(\alpha)}{2f'(\alpha)} = \dfrac{\varepsilon \sin \alpha}{2(1 - \varepsilon \cos \alpha)}$ ■

Problem 56 (Gautschi, Ch.4, 23, pag.253) *(a) Derive the iteration that results by applying Newton's method to $f(x) := x^3 - a = 0$ to compute the cube root $\alpha = a^{\frac{1}{3}}$ of $a > 0$.*

(b) *Consider the equivalent equation $f_\lambda(x) = 0$ where $f_\lambda(x) = x^{3-\lambda} - ax^{-\lambda}$, and determine λ so that Newton's method converges cubically. Write down the resulting iteration in its simplest form.*

Solution. (a) $f(x) = x^3 - a$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x)} = \frac{1}{3}\left(2x_n + \frac{a}{x_n^2}\right)$$

(b) $\varphi(x) = x - \frac{f(x)}{f'(x)} = \left(1 - \frac{x^{3-\lambda} - ax^{-\lambda}}{x^{3-\lambda}(3-\lambda) + ax^{-\lambda}\lambda}\right)x$

$\alpha = a^{1/3}$

$$\varphi'(\alpha) = 0, \quad \varphi''(\alpha) = 0, \quad \varphi'''(\alpha) \neq 0$$

$$\varphi''(\alpha) = 0 \Rightarrow -2\frac{-1+\lambda}{a^{\frac{1}{3}}} = 0 \Rightarrow \lambda = 1$$

$$f''(\alpha) = 0$$

After an usual algebraic manipulation we have

$$\varphi(x) = \frac{x(x^3 + 2a)}{2x^3 + a}$$

or

$$x_{n+1} = \frac{x_n(x_n^3 + 2a)}{2x_n^3 + a} = \frac{1}{2}\frac{x_n\left(x_n^3 + \frac{a}{2} + \frac{3a}{2}\right)}{x_n^3 + \frac{a}{2}}$$

$$= \frac{1}{2}\left(x_n + \frac{2ax_n}{2x_n^3 + a}\right)$$

■

Problem 57 (Gautschi, Ch.4, 36, pag.256) *Show that*

$$x_{n+1} = \frac{x_n(x_n^2 + 3a)}{3x_n^2 + a}$$

is a method for computing $\alpha = \sqrt{a}$, which converges cubically to α (for suitable x_0). Determine the asymptotic error constant.

Solution. Let

$$\varphi(x) = \frac{x(x^2+3a)}{3x^2+a}$$

$$\varphi(\sqrt{a}) = \sqrt{a}$$

$$\varphi'(x) = 3\frac{3x^4+a^2}{(3x^2+a)^2} > 0$$

$$\varphi'(\sqrt{a}) = 0$$

$$\varphi''(\sqrt{a}) = 0$$

$$|\varphi'(x)| < 1$$

$$\varphi'''(\sqrt{a}) = \frac{3}{2a}$$

$$\varphi'(x) - 1 = \frac{-2a(3x^2-a)}{(3x^2+a)^2} < 0$$

$$c = \frac{1}{4a}$$

$$3x^2 - a > 0$$

$$x_{1,2} = \pm\sqrt{\frac{a}{3}}$$

$$x \in \left(\left(-\infty, -\sqrt{\frac{a}{3}}\right) \cup \left(\sqrt{\frac{a}{3}}, \infty\right)\right) \cap \mathbb{R}_+^2$$

$$x_0 \in \left(\sqrt{\frac{a}{3}}, \infty\right)$$

■

Problem 58 (Gautschi, Ch.4, 37, pag.256) *Consider the fixed point iteration*

$$x_{n+1} = \varphi(x_n), \quad n \in \mathbb{N}$$

where

$$\varphi(x) = Ax + Bx^2 + Cx^3.$$

(a) *Given a positive number α, determine the constants A, B, C, such that the iteration converges locally to $1/\alpha$ with order $p = 3$. (This will give a cubically convergent method for computing the reciprocal $1/\alpha$ of α, which uses only addition, subtraction and multiplication).*

(b) Determine the precise condition on the initial error $\varepsilon_0 = x_0 - \dfrac{1}{\alpha}$ for the iteration to converge.

Solution. $p = 3$ implies

$$\varphi\left(\frac{1}{\alpha}\right) = A\frac{1}{\alpha} + B\frac{1}{\alpha^2} + C\frac{1}{\alpha^3} = \frac{1}{\alpha}$$

$$\varphi'\left(\frac{1}{\alpha}\right) = A + 2B\frac{1}{\alpha} + 3C\frac{1}{\alpha^2} = 0$$

$$\varphi''\left(\frac{1}{\alpha}\right) = 2B + 6C\frac{1}{\alpha} = 0$$

The solutions are

$$A = 3, \quad B = -3\alpha, \quad C = \alpha^2$$

(b) $|\varphi'(x)| < 1 \Rightarrow |3 - 6\alpha x + 3\alpha^2 x^2| < 1$

$$x_0 \in \left(\frac{1}{\alpha}\left(1 - \frac{\sqrt{3}}{3}\right), \frac{1}{\alpha}\left(1 + \frac{\sqrt{3}}{3}\right)\right)$$

■

Problem 59 (Gautschi, Ch.4, 43, pag.258) *Let $p(t)$ be a monic polynomial of degree n. Let $x \in \mathbb{C}^n$ and define*

$$f_\nu(x) = p[x_1, x_2, \ldots, x_\nu], \quad \nu = 1, 2, \ldots, n,$$

to be the divided difference of p relative to the coordinates x_μ of x. Consider the system of equations

$$f(x) = 0, \quad [f(x)]^T = [f_1(x), f_2(x), \ldots, f_n(x)].$$

(a) Let $\alpha^T = [\alpha_1, \alpha_2, \ldots, \alpha_n]$ be the zeros of p. Show that α is, except for a permutation of the components, the unique solution of $f(x) = 0$.

(Hint. Use Newton's formula of interpolation).

(b) Show that

$$\frac{\partial}{\partial x_0} g[x_0, x_1, \ldots, x_n] = g[x_0, x_0, x_1, \ldots, x_n]$$

assuming that g is a function differentiable at x_0. What about the partial derivatives with respect to other variable?

(c) *Describe the application of Newton's iterative method to the system of nonlinear equations $f(x) = 0$, given at point (a).*

(d) *Discuss to what extent the procedure in (a) and (c) is valid for non-polynomial functions p.*

Solution. (a) The nonlinear system is equivalent to

$$\begin{cases} p[x_1] = 0 \\ p[x_1, x_2] = 0 \\ \dots \\ p[x_1, x_2, \dots, x_n] = 0 \end{cases}$$

Newton's formula implies

$$p(x) = p[\alpha_1] + (x - \alpha_1)p[\alpha_1, \alpha_2] + \cdots + (x - \alpha_1)\dots(x - \alpha_{n-1})p[\alpha_1, \dots, \alpha_n], \tag{4.3}$$

since p is a polynomial.

$\alpha_1, \dots, \alpha_n$ roots of p

$$\begin{cases} 0 = p(\alpha_1) = p[\alpha_1] \Rightarrow p[\alpha_1] = 0 \\ 0 = p(\alpha_1) = p[\alpha_1] + (\alpha_2 - \alpha_1)p[\alpha_1, \alpha_2] \Rightarrow p[\alpha_1, \alpha_2] = 0 \\ \dots \\ 0 = p(\alpha_n) = p[\alpha_1] + (\alpha_n - \alpha_1)p[\alpha_1, \alpha_2] + \cdots + \\ +(\alpha_n - \alpha_1)\dots(\alpha_n - \alpha_{n-1})p[\alpha_1, \alpha_2, \dots, \alpha_n] \Rightarrow p[\alpha_1, \alpha_2, \dots, \alpha_n] = 0 \end{cases}$$

so $[\alpha_1, \alpha_2, \dots, \alpha_n]^T$ is a solution of $f(x) = 0$.

(b) $$\frac{g[x_0 + h, x_1, \dots, x_n] - g[x_0, x_1, \dots, x_n]}{h}$$

$$= g[x_0 + h, x_0, x_1, \dots, x_n] \to g[x_0, x_0, x_1, \dots, x_n]$$

Thus,

$$\frac{\partial}{\partial x_0} g[x_0, x_1, \dots, x_n] = g[x_0, x_0, x_1, \dots, x_n]$$

(b) The divided differences could be computed columnwise.

(c) Now applying Newton's method to the system $f(x) = 0$, we have

$$x^{(k+1)} = x^{(k)} - [f'(x^{(k)})]^{-1} f(x^{(k)})$$

But

$$f'(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_n} \\ \dots & \dots & \dots & \dots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \dots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

$$\begin{bmatrix} p[x_1,x_1] & 0 & 0 & \dots & 0 \\ p[x_1,x_1,x_2] & p[x_1,x_2,x_2] & 0 & \dots & 0 \\ p[x_1,x_1,x_2,x_3] & p[x_1,x_2,x_2,x_3] & p[x_1,x_2,x_3,x_3] & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ p[x_1,x_1,x_2,\dots,x_n] & p[x_1,x_2,x_2,\dots,x_n] & p[x_1,x_2,x_3,x_3,\dots,x_n] & \dots & p[x_1,x_2,\dots,x_n,x_n] \end{bmatrix}$$

and

$$f(x) = [p[x_1], p[x_1, x_2], \dots, p[x_1, \dots, x_n]]^T$$

(d) If p is a nonpolynomial function

$$p(x) = p[\alpha_1] + (x - \alpha_1)p[\alpha_1, \alpha_2] + \cdots + (x - \alpha_1)\dots(x - \alpha_{n-1})p[\alpha_1, \dots, \alpha_n]$$

$$+(x - \alpha_1)\dots(x - \alpha_n)p[x, x_1, \dots, x_n]$$

If $\alpha_1, \alpha_2, \dots, \alpha_n$ are zeros of the remainder vanishes, and the procedure is valid. ■

Problem 60 *(Gautschi, Ch.4, 44, pag.258)*

For the equation $f(x) = 0$ define

$$y^{[0]}(x) = x$$

$$y^{[1]}(x) = \frac{1}{f'(x)}$$

$$\dots$$

$$y^{[m]}(x) = \frac{1}{f'(x)} \frac{d}{dx} y^{[m-1]}(x), \quad m = 2, 3, \dots$$

Consider the iteration function

$$\varphi_r(x) := \sum_{m=0}^{r} (-1)^m \frac{y^{[m]}(x)}{m!} [f(x)]^m$$

When $r = 1$ this is the iteration function for Newton's method. Show that $\varphi_r(x)$ defines an iteration $x_{n+1} = \varphi_r(x_n)$, $n = 0, 1, 2, \dots$ converging locally with exact order $p = r + 1$ to a root α of the equation if $y^{[r+1]}(\alpha)f'(\alpha) \neq 0$.

Solution. $f'(\alpha) \neq 0 \Rightarrow \exists g = f^{-1}$ on a neighbor $V(\alpha)$ of α

$$g(y) = \sum_{m=0}^{r} \frac{(y - f(x))^m}{m!} g^{(m)}(f(y)) + \frac{[y - f(x)]^{r+1}}{(r+1)!} g^{(r+1)}(y - f(x))$$

(Taylor expansion around $f(x)$)

$$g(0) = f^{-1}(f(\alpha)) = \alpha$$

$$\alpha \approx g(0) = \sum_{m=0}^{r} \frac{(-1)^m}{m!} g^{(m)}(f(x)) + \frac{(-1)^{m+1}}{(m+1)!}[f(x)]^{m+1} g^{(m+1)}((1-\theta)f(x))$$

But

$$[g^{(m)}(f(x))']' = g^{(m+1)}(f(x))f'(x)$$

so

$$g^{(m+1)}(f(x)) = \frac{1}{f'(x)} \frac{d}{dx}[g^{(m)}(f(x))]$$

Now

$$y(x) = g(f(x))$$

$$y^{[k]} = g^{(k)}(f(x)), \quad k = \overline{0, r}$$

$$\alpha - \varphi_r(x) = \frac{(-1)^{r+1}}{(r+1)!}[f(x)]^{r+1} y^{(r+1)}((1-\theta)f(x))$$

$$\alpha - x_{k+1} = \frac{(-1)^{r+1}}{(r+1)!}[f(x_k) - f(\alpha)]^{r+1} y^{[r+1]}((1-\theta)x_k)$$

$$\frac{(-1)^{r+1}}{(r+1)!}(x_k - \alpha)^{r+1}[f'(\xi)]^{r+1} y^{[r+1]}((1-\theta)x_k)$$

$$\frac{|\alpha - x_{k+1}|}{|\alpha - x_k|^{r+1}} = \frac{1}{(r+1)!}[f'(\xi)]^{r+1} y^{[r+1]}((1-\theta)x_k)$$

$$\to \frac{1}{(r+1)!}[f'(\alpha)]^{r+1} y^{[r+1]}(\alpha)$$

■

Problem 61 *(Gautschi, Ch.4, 39, p.257)*

Let α be a simple zero of f and $f \in C^p$ near α, where $p \geq 3$. Show: if $f''(\alpha) = \cdots = f^{(p-1)}(\alpha) = 0$, $f^{(p)}(\alpha) \neq 0$, then Newton's method applied to $f(x) = 0$ converges to α locally with order p. Determine the asymptotic error constant.

Solution. $\varphi(x) = x - \dfrac{f(x)}{f'(x)}$

$$\varphi'(x) = 1 - \frac{f'^2(x) - f''(x)f(x)}{f'^2(x)} = f(x)\frac{f''(x)}{f'^2(x)}$$

$$\varphi^{(k+1)}(x) = \sum_{i=1}^{k} \binom{k}{i} f^{(i)}(x) \left(\frac{f''(x)}{f'^2(x)} \right)^{(k-i)} \tag{4.4}$$

$k = 1$

$$\varphi''(x) = f(x) \left(\frac{f''(x)}{f'^2(x)} \right)' + f'(x) \frac{f''(x)}{f'^2(x)}$$

$\varphi''(\alpha) = 0$ if $f''(\alpha) = 0$

$k = p - 2$

$$\varphi^{p-1}(x) = \sum_{i=0}^{p-2} \binom{p-2}{i} f^{(i)}(x) \left(\frac{f''(x)}{f'^2(i)} \right)^{(p-i-2)}$$

$$= f(x) \left[\frac{f''(x)}{f'^2(x)} \right]^{(p-1)} + f'(x) \left[\frac{f''(x)}{f'^2(x)} \right]^{p-2}$$

$$+ \sum_{i=2}^{p-1} \binom{p-1}{i} f^{(i)}(x) \left(\frac{f''(x)}{f'^2(x)} \right)^{(p+1)}$$

for $2 \le k \le p-1$ and $x = \alpha$. Since $f^{(k)}(\alpha) = 0$ all terms in (4.4) vanish except the second

$$\binom{k}{1} f'(x) \left[\frac{f''(x)}{f'^2(x)} \right]^{(k-1)}.$$

But the expansion of this term contains derivatives of order at least 2 so it also vanishes.

For $k = p$ the second term does not vanish

$$\varphi^{(p)}(\alpha) \neq 0$$

$$c = \frac{\varphi^{(p)}(\alpha)}{p!}$$

$$\varphi^{(p)}(x) = \left(f(x) \frac{f''(x)}{f'^2(x)} \right)^{(p-1)} = f(x) \left[\frac{f''(x)}{f'^2(x)} \right]^{(p-1)}$$

$$+ (p-1) f'(x) \left[\frac{f''(x)}{f'^2(x)} \right]^{(p-2)} + \sum_{k=2}^{p-1} \binom{p-1}{k} f^{(k)}(x) \left[\frac{f''(x)}{f'^2(x)} \right]^{(p-1-k)}$$

Only the second term does not vanish for $p = \alpha$, so

$$c = \frac{p-1}{p!} f'(x) \left[\frac{f''(x)}{f'^2(x)} \right]^{(p-2)}_{x=\alpha}$$

But

$$\left[\frac{f''(x)}{f'^2(x)}\right]^{(p-2)} = \left[f''(x)\frac{1}{f'^2(x)}\right]^{(p-2)} = f^{(p)}(x)\frac{1}{f'^2(x)}$$

$$+\sum_{k=1}^{p-2}\binom{p-2}{k} f^{(p-k)}(x)\left(\frac{1}{f'^2(x)}\right)^n$$

Only the first term does not vanish for $x=\alpha$ so

$$c = \frac{p-1}{p!}\frac{f^{(p)}(\alpha)}{f'(\alpha)}.$$

■

Problem 62 *(Gautschi, Ch.4, 40, pag.257)*
The iteration

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n) - \frac{1}{2}f''(x_n)\frac{f(x_n)}{f'(x_n)}}, \quad n = 0, 1, 2, \ldots$$

for solving equation $f(x) = 0$ is known as Halley's method.

(a) Interpret Halley's method geometrically as the intersection with the x-axis of a hyperbola with asymptotes parallel to the $x-$ and $y-$ axes that is osculatory to the curve $u = f(x)$ at $x = x_n$ (i.e. is tangent to the curve at this point and has the same curvature there).

(b) Show that the method can alternatively be interpreted as applying Newton's method to the equation $g(x) = 0$, $g(x) = f(x)/\sqrt{f'(x)}$.

(c) Assuming α is a simple root of the equation, and $x_n \to \alpha$ as $n \to \infty$, show that convergence is exactly cubic, unless the "Schwarzian derivative"

$$(Sf)(x) := \frac{f'''(x)}{f'(x)} - \frac{3}{2}\left(\frac{f''(x)}{f'(x)}\right)^2$$

vanishes at $x = \alpha$, in which case the order of convergence is larger than three.

(d) Is Halley's method more efficient than Newton's method as measured in terms of efficiency index?

(e) How does Halley's method look in the case $f(x) = x^\lambda - a$, $a > 0$?

Solution. Hyperbola equation is

$$h(x) = b + \frac{c}{x-a}$$

Hyperbola is osculatory to $y = f(x)$ implies

$$\begin{cases} h(x_n) = f(x_n) \\ h'(x_n) = f'(x_n) \\ h''(x_n) = f''(x_n) \end{cases} \Leftrightarrow \begin{cases} b + \dfrac{c}{x_n - a} = f(x_n) \\[2ex] -\dfrac{c}{(x_n-a)^2} = f'(x_n) \\[2ex] \dfrac{2c}{(x_n-a)^3} = f''(x_n) \end{cases}$$

The solution is

$$a = x + \frac{2f'(x_n)}{f''(x_n)}$$

$$b = f(x_n) - 2\frac{f'^2(x_n)}{f''(x_n)}$$

$$c = -4\frac{f'^3(x_n)}{f''^2(x_n)}$$

Hyperbola's intersection with x axis is

$$x_{n+1} = x_n + \frac{2f'(x_n)}{f''(x_n)} + \frac{4f'^3(x_n)}{f''^2(x_n)\left(f(x_n) - \dfrac{2f'^2(x_n)}{f''(x_n)}\right)}$$

$$= x_n + \frac{2f'(x_n)}{f''(x_n)} + \frac{4f'^3(x_n)}{f''(x_n)[f(x_n)f''(x_n) - 2f'^2(x_n)]}$$

$$= x_n - \frac{2f(x_n)f'(x_n)}{2f'^2(x_n) - f(x_n)f''(x_n)}$$

$$= x_n - \frac{f(x_n)}{f'(x_n) - \dfrac{1}{2}f''(x_n)\dfrac{f(x_n)}{f'(x_n)}}$$

(b) $g(x) = \dfrac{f(x)}{\sqrt{f'(x)}}$

$$g'(x) = \sqrt{f'(x)} - \frac{1}{2}\frac{f(x)f'^2(x)}{\sqrt{f'^3(x)}}$$

$$= \frac{1}{2}\frac{f'^2(x) - f(x)f'^2(x)}{f'(x)\sqrt{f'(x)}}$$

$$\varphi(x) = x - \frac{g(x)}{g'(x)} = x - 2\frac{f(x)f'(x)}{-2f'^2(x) + f(x)f''(x)}$$

$$= x - \frac{f(x)}{f'(x) - \dfrac{1}{2}f''(x)\dfrac{f(x)}{f'(x)}}$$

(c) Using problem ??

$$g''(x) = -\frac{1}{4}\frac{f(x)[3f''^2(x) + 2f'f'''(x)]}{[f'(x)]^{5/2}}$$

$g''(\alpha) = 0$, we conclude that order $p \geq 3$

$$g'''(x) = \left(-\frac{15}{8}\frac{f''^3(x)}{[f'(x)]^{\frac{7}{2}}} + \frac{\frac{9}{4}f''(x)f'''(x)}{[f'(x)]^{\frac{5}{2}}} - \frac{1}{2}\frac{f'''(x)}{[f'(x)]^{\frac{3}{2}}}\right) f(x)$$

$$+\frac{\frac{3}{4}f''^2(x)}{[f'(x)]^{\frac{3}{2}}} - \frac{1}{2}\frac{f'''(x)}{[f'(x)]^{1/2}}$$

The first term vanishes for $x = \alpha$. The exact order is $p = 3$. When

$$\frac{1}{2}\frac{1}{\sqrt{f'(x)}}\left[\frac{f'''(x)}{f'(x)} - \frac{3}{2}\left(\frac{f''(x)}{f'(x)}\right)^2\right] \neq 0$$

vanishes for $x = \alpha$ the order is larger than 3.

(d) $2^{\frac{1}{2}} \approx 1.414213562$

$3^{\frac{1}{3}} \approx 1.442249570$

The efficiency index of Halley's method is larger than that of Newton's method.

(e) For $f(x) = x^\lambda - a$ one gets

$$x_{n+1} = \frac{x_n[(\lambda - 1)x_n^\lambda + (\lambda + 1)a]}{(\lambda + 1)x_n^\lambda + (\lambda - 1)a}$$

■

Problem 63 (Gregory, 1672 and Gautschi, Ch.4, p.31, pag.255) *For an integer $n \geq 1$, consider the equation*

$$f(x) = 0, \quad f(x) = x^{n+1} - b^n x + ab^n, \quad a > 0,\ b > 0.$$

(a) *Prove that the equation has exactly two distinct positive roots if and only if*

$$a < \frac{n}{(n+1)^{1+\frac{1}{n}}} b.$$

*(*Hint*. Analyze the convexity of f.)*

(b) *Assuming that the conditions in (a) holds, show that Newton's method converges to the smaller positive root, when started at $x_0 = a$ and to the larger one, when started at $x_0 = b$.*

Solution. (a) $f(a) = a^{n+1} - ab^n + ab^n > 0$

$$f(b) = b^{n+1} - b^{n+1} + ab^n > 0$$

$$f'(x) = (n+1)x^n - b^n$$

$$f''(x) = (n+1)nx^{n-1} > 0 \text{ for } x > 0$$

$$f'(x) = 0 \Rightarrow x_0 = \frac{b}{\sqrt[n]{n+1}} = \frac{b}{(n+1)^{\frac{1}{n}}}$$

$$f(x_0) = \frac{-nb^{n+1}}{(n+1)^{1+\frac{1}{n}}} + ab^n = b^n \left(-\frac{nb}{(n+1)^{1+\frac{1}{n}}} + a \right)$$

$$f(x_0) < 0 \Rightarrow a < \frac{nb}{(n+1)^{1+\frac{1}{n}}} \tag{4.5}$$

(4.5) $\Rightarrow f$ has two distinct positive root

h has two distinct root $\Rightarrow f'(x_0) < 0 \Rightarrow$ (4.5)

(b) $x_0 = a$, $f(x_0)f''(x_0) > 0$

(x_n) convergent x_n increasing, and bounded by the smallest positive root

$x_0 = b$, $f(x_0)f''(x_0) > 0$

(x_n) decreasing, bounded by the largest positive root $\Rightarrow (x_n)$ convergent.

■

Problem 64 *Given an iterative method of order p and asymptotic error constant $c \neq 0$, define a new iterative method consisting of m consecutive steps of the given method. Determine the order of this new iterative method and its asymptotic error constant. Hence justify the definition of the efficiency index.*

Solution. Denote by en the error of the given method after n steps. Since the method has order p and asymptotic error constant $c \neq 0$, we have

$$\frac{e_{n+1}}{e_n^p} \to c, \text{ as } n \to \infty.$$

Now,

$$\frac{e_{n+p}}{e_n^{p^m}} = \prod_{k=1}^{m} \left(\frac{e_{n+k}}{e_{n+k-1}^p} \right)^{p^{m-k}} =$$
$$= \left(\frac{e_{n+1}}{e_n^p} \right)^{p^{m-1}} \left(\frac{e_{n+2}}{e_{n+1}^p} \right)^{p^{m-2}} \cdots \left(\frac{e_{n+m}}{e_{n+m-1}^p} \right)^{p^{m-m}},$$

since each numerator on the far right cancels against the next denominator, leaving precisely the ratio on the far left. Therefore, when $n \to \infty$,

$$\frac{e_{n+p}}{e_n^{p^m}} \longrightarrow c^{p^{m-1}+p^{m-2}+\cdots+p+1} = c^{\frac{p^m-1}{p-1}}$$

so that the new method has order p^m and asymptotic error constant $c^{\frac{p^m-1}{p-1}}$ ($= c^m$ if $p = 1$). If we consider one step of the original method as 1 "operation", then its efficiency index is p. The "new method" then requires m operations per step, hence its efficiency index is $(p^m)^{1/m} = p$, the same as the original method, as it should be. ■
Proof.

Problem 65 *Let $\{x_n\}$ be a sequence converging to α. Suppose the errors $e_n = |x_n - \alpha|$ satisfy $e_{n+1} \leq M e_n^2 e_{n-1}$ for some constant $M > 0$. What can be said about the order of convergence?*

■
Proof. Define $E_n = M^{1/2} e_n$. Then

$$E_{n+1} \leq E_n^2 E_{n-1}, \tag{*}$$

To guess the order of convergence, assume we have equality in (*). Taking logarithms,

$$y_n = \ln \frac{1}{E_n},$$

then gives $y_{n+1} = 2y_n + y_{n-1}$, a constant-coefficient difference equation whose characteristic equation is $t^2 - 2t - 1 = 0$. There are two solutions t_i^n,

$i = 1, 2$, corresponding to the two roots $t_{1,2} = 1 \pm \sqrt{2}$. Only the first tends to ∞ as $n \to \infty$. Therefore,

$$y_n = c\left(1+\sqrt{2}\right)^n$$

for some constant $c > 0$. There follows

$$\begin{aligned}
\ln \frac{1}{E_n} &= c\left(1+\sqrt{2}\right)^n \\
E_n &= e^{-c\left(1+\sqrt{2}\right)^n} \\
\frac{E_{n+1}}{E_n^{1+\sqrt{2}}} &= \frac{e^{-c\left(1+\sqrt{2}\right)^{n+1}}}{\left[e^{-c\left(1+\sqrt{2}\right)^n}\right]^{1+\sqrt{2}}} = 1.
\end{aligned}$$

Thus, E_n, and hence also e_n, converges to zero with order $p = 1 + \sqrt{2}$.

Assume now (*) with inequality as shown, and let $p = 1 + \sqrt{2}$. Since

$$p^2 = 2p + 1,$$

one proves by induction that

$$E_n \le E^{p^n}, \quad E = \max\left(E_0, E_1^{\frac{1}{p}}\right).$$

Therefore,

$$e_n = M^{-1/2} E_n \le M^{-1/2} E^{p^n} =: \varepsilon_n,$$

and

$$\frac{e_{n+1}}{e_n^p} = \frac{M^{-\frac{1}{2}} E^{p^{n+1}}}{M^{-\frac{p}{2}} \left(E^{p^n}\right)^p} = M^{\frac{p-1}{2}}$$

showing that ε_n converges to zero with order p, hence e_n at least with order p. ■

Problem 66 *Consider the equation*

$$x = e^{-x}.$$

(a) Show that there is a unique real root α and determine an interval containing it.

(b) Show that the fixed point iteration $x_{n+1} = e^{-x_n}$, $n = 0, 1, 2, \ldots$, converges locally to α and determine the asymptotic error constant.

(c) *Illustrate graphically that the iteration in (b) actually converges globally, that is, for arbitrary $x_0 > 0$. Then prove it.*

(d) *An equivalent equation is*

$$x = \ln \frac{1}{x}.$$

Does the iteration $x_{n+1} = ln \frac{1}{x_n}$ also converge locally? Explain.

Solution.

(a) Letting $f(x) = x - e^{-x}$, we have $f\prime(x) = 1 + e^{-x} > 1$ for all real x. Consequently, f increases monotonically on $\mathbb{R}$ from $-\infty$ to ∞, hence has exactly one real zero, α. Given that $f(0) = -1$ and $f(1) = 1 - e^{-1} > 0$, we have $0 < \alpha < 1$.

(b) The fixed point iteration is $x_{n+1} = \varphi(x_n)$ with $\varphi(x) = e^{-x}$. Clearly, $\alpha = \varphi(\alpha)$, and $\varphi'(\alpha) = e^{-\alpha}$, hence $0 < |\varphi(\alpha)| = e^{-\alpha} < 1$. Therefore, we have local convergence, the asymptotic error constant being $c = -e^{-\alpha}$.

(c) For definiteness, assume $x_0 > \alpha$. Then the fixed point iteration behaves as indicated in the figure 4.1: the iterates "spiral" clockwise around, and into, the fixed point . The same spiraling takes place if $0 < x_0 < \alpha$ (simply relabel x_1 in the figure as x_0).

Proof of global convergence. From the mean value theorem of calculus, applied to the function e^{-x}, one has

$$|x_{n+1} - \alpha| = |e^{-x_n} - e^{-\alpha}| = e^{-\xi_n}|x_n - \alpha|,$$

where ξ_n is strictly between α and x_n. Letting $\mu = \min(x_0, x_1)$, it is clear from the graph in Figure **??** that $\mu > 0$ and $x_n \geq \mu$ (all $n \geq 0$), $\alpha > \mu$. Therefore, ξ_n being stricly between α and x_n, we have that $\xi_n > \mu$ for all n, hence

$$|x_{n+1} - \alpha| < e^{-\mu}|x_n - \alpha|.$$

Applying this repeatedly gives $|x_n - \alpha| < e^{-\mu n}|x_0 - \alpha| \to 0$ as $n \to \infty$.

(d) Here, $x_{n+1} = \psi(x_n)$, where $\psi(x) = \ln \frac{1}{x}$. Since $|\psi'(\alpha)| = \frac{1}{\alpha} > 1$, we cannot have local convergence to α if $x_0 \neq \alpha$.

■

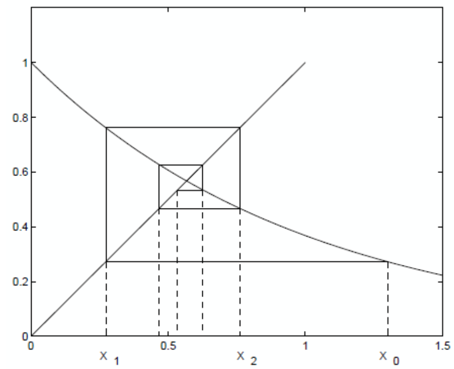

Figure 4.1: Problema 66

Problem 67 *Consider the equation*

$$\tan x + \lambda x = 0, \quad 0 < \lambda < 1.$$

(a) Show graphically, as simply as possible, that in the interval $\left[\frac{1}{2}\pi, \pi\right]$ *there is exactly one root* α*.*

(b) Does Newton's method converge to the root $\alpha \in \left[\frac{1}{2}\pi, \pi\right]$*, if the initial approximation is taken to be* $x_0 = \pi$*? Justify your answer.*

Solution.

(a) The graphs of $y = \tan x$ and $y = -\lambda x$ for $x > 0$ intersect for the first time at a point whose abscissa, a root of the equation, is between $\frac{1}{2}\pi$ and π. This is the only root in that interval.

(b) With $f(x) = \tan x + x$, we have, on $\left[\frac{1}{2}\pi, \pi\right]$,

$$\begin{aligned} f\left(\frac{\pi}{2} + 0\right) &= -\infty, \ f(\pi) = \lambda\pi \\ f'(x) &= \frac{1}{\cos^2 x} + \lambda > 0, \\ f''(x) &= \frac{d}{dx}\left(\frac{1}{\cos^2 x}\right) = \frac{2}{\cos^3 x}\sin x < 0, \end{aligned}$$

so that on this interval f is monotonically increasing and concave. If Newton's method is started at the right endpoint, $x_0 = \pi$, then it will converge monotonically increasing if $x_1 > \frac{\pi}{2}$. This is true, since

$$x_1 = \pi - \frac{f(\pi)}{f'(\pi)} = \frac{\pi}{1+\lambda} > \frac{\pi}{2},$$

since $\lambda \in [0,1]$.

■

Problem 68 *(a) If $A > 0$, then $\alpha = \sqrt{A}$ is a root of either equation*

$$x^2 - A = 0, \qquad \frac{A}{x^2} - 1 = 0.$$

Explain why Newton's method applied to the first equation converges for arbitrary starting value $x_0 > 0$, whereas the same method applied to the second equation produces positive iterates x_n converging to α only if x_0 is in some interval $0 < x_0 < b$. Determine b.

(b) Do the same as (a), but for the cube root $\sqrt[3]{A}$ and the equations $x^3 - A = 0$, $\frac{A}{x^3} - 1 = 0$.

Solution.

(a) In the first case, the function $f(x) = x^2 - A$ is convex on $\mathbb{R}_+$ and increases monotonically from 0 to ∞. Therefore, if $x_0 > \alpha$, then (x_n) converges monotonically decreasing to α. If $0 < x_0 < \alpha$, then $x_1 > \alpha$, and the same conclusion holds for $n > 1$. In the second case, $f(x) = \frac{A}{x^2} - 1$ is again convex on $\mathbb{R}_+$, but decreases from ∞ to -1. If $0 < x_0 < \alpha$, then (x_n) converges monotonically increasing to α. If $x_0 > \alpha$, we must make sure that $x_1 > 0$, which means that

$$x_1 = x_0 - \frac{\frac{A}{x_0^2} - 1}{-2\frac{A}{x_0^3}} > 0, \quad x_0 + x_0\frac{A - x_0^2}{2A} > 0$$

$$x_0\left(3A - x_0^2\right) > 0,\ x_0 < \sqrt{3A} =: b.$$

(b) For the first equation, the reasoning is the same as in (a), and similar for the second equation, the condition $x_1 > 0$ now becoming

$$x_0(4A - x_0^3) > 0, \quad x_0 < \sqrt[3]{4A} =: b.$$

■

Problem 69 *Consider the two (equivalent) equations*

$$(A)\ x\ln x - 1 = 0; \quad (B)\ \ln x - \frac{1}{x} = 0.$$

(a) Show that there is exactly one positive root and find a rough interval containing it.

(b) For both (A) and (B), determine the largest interval on which Newton's method converges. (Hint: investigate the convexity of the functions involved.)

(c) Which of the two Newton iterations converges asymptotically faster?

Solution.

(a) The graphs of $y = \ln x$ and $y = 1/x$ clearly intersect at exactly one point, whose abscissa is larger than 1 (obviously) and less than 2 (since $\ln 2 > 1/2$).

(b) Let first $f(x) = x\ln x - 1$. Then $f'(x) = \ln x + 1$, $f''(x) = \frac{1}{x}$, so that f is convex on $\mathbb{R}_+$. For any x_0 in the interval $(0, e^{-1})$, where f is monotonically decreasing, Newton's method produces a negative x_1, which is unacceptable. On the other hand, Newton's method, by convexity of f, converges monotonically decreasing (except, possibly, for the first step) for any x_0 in (e^{-1}, ∞). Let now $g(x) = \ln x - \frac{1}{x}$. Here, $g'(x) = x^{-2}(x+1)$, $g''(x) = -x^{-3}(x+2)$, so that g increases monotonically from $-\infty$ to $+\infty$ and is concave on $\mathbb{R}+$. For any $x_0 < \alpha$, therefore, Newton's method converges monotonically increasing. If $x_0 > \alpha$, one must ensure that $x_1 > 0$. Since

$$x_1 = x_0 - \frac{\ln x_0 - x_0^{-1}}{x_0^{-2}(x_0+1)} = x_0 \frac{x_0 + 2 - x_0 \ln x_0}{x_0 + 1},$$

we thus must have $x_0 + 2 - x_0 \ln x_0 > 0$, i.e., $x_0 < x_*$ where

$$x_* \ln x_* - x_* - 2 = 0.$$

This has a unique solution between 4 and 5, which can be obtained in turn by Newton's method. The result is $x = 4.319136566\ldots$.

(c) The respective asymptotic error constants are

$$c_f = \left.\frac{f''(x)}{2f'(x)}\right|_{x=\alpha} = \left.\frac{1}{2x\,(\ln x + 1)}\right|_{x=\alpha} = \frac{1}{2\,(\alpha+1)}.$$

$$c_g = \left.\frac{g''(x)}{2g'(x)}\right|_{x=\alpha} = -\frac{\alpha+2}{2\alpha(\alpha+1)}$$

We have

$$\frac{c_f}{|c_g|} = \frac{1}{2\,(\alpha+1)} \cdot \frac{2\alpha(\alpha+1)}{\alpha+2} = \frac{1}{1+\frac{2}{a}}.$$

Since $1+\frac{2}{a} > 2$, we have $c_f < 1/2|c_g|$, so that Newton's method for (A) converges asymptotically faster by more than a factor of 2.

■

Problem 70 *The equation*

$$\cos x \cosh x - 1 = 0$$

has exactly two roots $\alpha_n < \beta_n$ *in each interval* $\left[-\frac{\pi}{2}+2n\pi, \frac{\pi}{2}+2n\pi\right]$, $n = 1, 2, 3, \ldots$ *Show that Newton's method applied to this equation converges to* α_n *when initialized by* $x_0 = -\frac{\pi}{2}+2n\pi$ *and to* β_n *when initialized by* $x_0 = \frac{\pi}{2}+2n\pi$.

Solution. We have

$$\begin{aligned} f(x) &= \cos x \cosh x - 1 \\ f'(x) &= \cos x \sinh x - \sin x \cosh x \\ f''(x) &= -2 \sin x \sinh x \end{aligned}$$

Clearly, $f''(x) > 0$ on $\left[-\frac{\pi}{2}+2n\pi, 2n\pi\right]$ and $f''(x) < 0$ on $\left[2n\pi, \frac{\pi}{2}+2n\pi\right]$. Furthermore, $f\left(-\frac{\pi}{2}+2n\pi\right) = f\left(\frac{\pi}{2}+2n\pi\right) = -1$ and $f(2n\pi) = \cosh(2n\pi) > 1$. Since f is convex on the first half of the interval $\left[-\frac{\pi}{2}+2n\pi, \frac{\pi}{2}+2n\pi\right]$, Newton's method started at the left endpoint converges monotonically decreasing (except for the first step) to α_n, provided the first iterate is to the left of the midpoint. This is the case since, with $x_0 = -\frac{\pi}{2}+2n\pi$, we have, for $n \geq 1$,

$$\begin{aligned} x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} &= -\frac{\pi}{2} + 2n\pi + \frac{1}{\cosh\left(-\frac{\pi}{2}+2n\pi\right)} \\ &< -\frac{\pi}{2} + 2n\pi + \frac{1}{\cosh\left(\frac{3\pi}{2}\right)} = 2n\pi - 1.55283... < 2n\pi. \end{aligned}$$

Since f is concave on the second half of the interval, Newton's method started at the right endpoint converges monotonically decreasing to β_n. ■

Problem 71 *Prove the theorem: Let α be a simple root of the equation $f(x) = 0$ and let $I_\varepsilon = \{x \in \mathbb{R} : |x - \alpha| < \varepsilon\}$. Assume that $f \in C^2[I_\varepsilon]$. Define*

$$M(\varepsilon) = \max_{s,t \in I_\varepsilon} \left| \frac{f''(s)}{2f'(t)} \right| \tag{4.6}$$

If ε is so small that

$$2\varepsilon M(\varepsilon) < 1 \tag{4.7}$$

then for every $x_0 \in I_\varepsilon$, Newton's method is well defined and converges quadratically to the only root $\alpha \in I_\varepsilon$. (The extra factor 2 in (4.7) comes from the requirement that $f'(x) \neq 0$ for $x \in I_\varepsilon$.)

Proof. By Taylor's theorem applied to f and f',

$$\begin{aligned} f(x) &= f(\alpha) + (x-\alpha)f'(\alpha) + \frac{1}{2}(x-\alpha)^2 f''(\xi) \\ &= (x-\alpha)f'(\alpha)\left[1 + (x-\alpha)\frac{f''(\xi)}{2f'(a)}\right], \\ f'(x) &= f'(\alpha) + (x-\alpha)f''(\xi_1) \\ &= f'(\alpha)\left[1 + (x-\alpha)\frac{f''(\xi_1)}{f'(\alpha)}\right] \end{aligned}$$

where ξ_1 and ξ_2 lie between α and x. If $x \in I_\varepsilon$ and $2\varepsilon M(\varepsilon) < 1$, then

$$\left|(x-\alpha)\frac{f''(\xi)}{2f'(a)}\right| \leq \varepsilon M(\varepsilon) < \frac{1}{2},$$

so that $f(x) \neq 0$ for $x = \alpha$. Likewise,

$$\left|(x-\alpha)\frac{f''(\xi_1)}{f'(\alpha)}\right| \leq 2\varepsilon M(\varepsilon) < 1,$$

so that also $f'(x) \neq 0$. Use

$$|x_{n+1} - \alpha| = (x_n - \alpha)^2 \frac{f[x_n, x_n, \alpha]}{f[x_n, x_n]} \tag{4.8}$$

Furthermore, $x_n \in I_\varepsilon$ implies by (4.8) that $|x_{n+1} - \alpha| < \varepsilon \cdot \varepsilon M(\varepsilon) < \frac{1}{2}\varepsilon$, in particular, $x_{n+1} \in I_\varepsilon$. Since $x_0 \in I_\varepsilon$ it follows that all $x_n \in I_\varepsilon$, and since $f'(x_n) \neq 0$, Newton's method is well defined. Finally, again by (4.8),

$$|x_{n+1} - \alpha| \leq |x_n - \alpha| \, \varepsilon M(\varepsilon), \qquad n = 1, 2, 3, \ldots,$$

giving

$$|x_n - \alpha| \leq [\varepsilon M(\varepsilon)]^n \, |x_0 - \alpha| \to 0 \text{ as } n \to \infty$$

since $\varepsilon M(\varepsilon) < \frac{1}{2}$. ■

Problem 72 *In the engineering of circular shafts the following equation is important for determining critical angular velocities:*

$$f(x) = 0, \quad f(x) = \tan x + \tanh x, \ x > 0.$$

(a) Show that there are infinitely many positive roots, exactly one, α_n, in each interval $\left[\left(n - \frac{1}{2}\right)\pi, n\pi\right]$, $n = 1, 2, 3, \ldots$

(b) Determine $\lim_{n\to\infty} (n\pi - \alpha_n)$.

(c) Discuss the convergence of Newton's method when started at $x_0 = n\pi$.

Solution.

(a) The graphs of $y = \tan x$ and $y = -\tanh x$ on $\mathbb{R}_+$ intersect infinitely often, exactly once in each interval $[(n - 1/2)\pi, n\pi]$, $n = 1, 2, 3, \ldots$. The respective abscissae α_n are the positive roots of the equation.

(b) Since $\tanh x \to 1$ când $x \to \infty$, the geometric discussion in (a) shows that $\alpha_n - n\pi \sim \tan^{-1}(-1) = -\tan^{-1}(1)$, hence $n\pi - \alpha_n \to \tan^{-1}(1) = \pi/4 = .785398\ldots$ as $n \to \infty$.

(c) On the interval $I_n = [(n - 1/2)\pi, n\pi]$ we have $f\left((n - 1/2)\pi\right) = -\infty$, $f(n\pi) = \tanh n\pi > 0$ and

$$\begin{aligned} f'(x) &= \tan^2 x - \tanh^2 x + 2 \\ f''(x) &= 2\tan x\left(\tan^2 x + 1\right) - 2\tanh x\left(1 - \tanh^2 x\right) \end{aligned}$$

Thus, f is monotonically increasing and concave on I_n. Newton's method will converge if started at the right endpoint, $x_0 = n\pi$, provided $x_1 > (n - 1/2)\pi$. This is indeed the case: since the function $u/(2 - u^2)$ on $[0, 1]$ increases from 0 to 1, we have

$$x_1 = n\pi - \frac{\tanh n\pi}{2 - \tanh^2 n\pi} > n\pi - 1 > n\pi - \frac{1}{2}\pi.$$

■

Problem 73 *The equation $f(x) = x^2 - 3x + 2 = 0$ has the roots 1 and 2. Written in fixed point form $x = \frac{1}{\omega}\left[x^2 - (3 - \omega)x + 2\right]$, $\omega \neq 0$, it suggests the iteration*

$$x_{n+1} = \frac{1}{\omega}\left[x_n^2 - (3 - \omega)x_n + 2\right], \quad n = 1, 2, \ldots \ (\omega \neq 0)$$

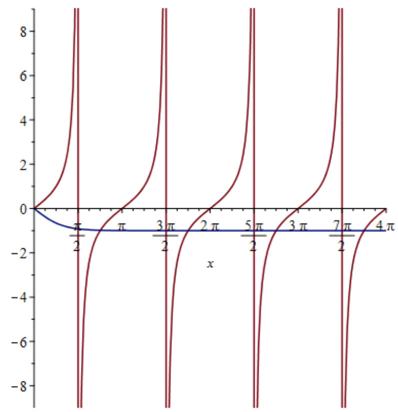

Figure 4.2: Problema 72

(a) *Identify as large an ω-interval as possible such that for any ω in this interval the iteration converges to 1 (when $x_0 \neq 1$ is suitably chosen).*

(b) *Do the same as (a), but for the root 2 (and $x_0 \neq 2$).*

(c) *For what value(s) of ω does the iteration converge quadratically to 1?*

(d) *Interpret the algorithm produced in (c) as a Newton iteration for some equation $F(x) = 0$, and exhibit F. Hence discuss for what initial values x_0 the method converges.*

Solution.

(a) (a) The algorithm is the fixed point iteration $x_{n+1} = \varphi(x_n)$, where $\varphi(x) = \frac{1}{\omega}\left[x^2 - (3-\omega)\,x + 2\right]$. Local convergence to 1 requires that $|\varphi'(1)| < 1$. Since

$$\varphi'(x) = \frac{1}{\omega}\left[2x - (3-\omega)\right],$$

this gives

$$\left|\varphi'(1)\right| = \left|\frac{\omega - 1}{\omega}\right| < 1 \Longrightarrow \frac{1}{2} < \omega < \infty.$$

(b) Similarly,

$$\left|\varphi'(2)\right| = \left|\frac{\omega + 1}{\omega}\right| < 1 \Longrightarrow \infty < \omega < -\frac{1}{2}.$$

(c) We have quadratic convergence to 1 precisely if $\varphi'(1) = 0$, that is, $\omega = 1$.

(d) The algorithm can be written in the form

$$x_{n+1} = x_n^2 - 2x_n + 2 = x_n - \left(3x_n - x_n^2 - 2\right) = x_n - \frac{F(x_n)}{F'(x_n)}$$

provided

$$\frac{F(x)}{F'(x)} = 3x - x^2 - 2 = -\left(x-1\right)\left(x-2\right)$$

or

$$\frac{F'(x)}{F(x)} = (\ln F)' = -\frac{1}{\left(x-1\right)\left(x-2\right)} = \frac{1}{x-1} - \frac{1}{x-2}$$

Integration followed by exponentiation gives

$$F(x) = C \log \frac{x-1}{x-2}$$

From the graph of the function F (we may set the constant equal to 1), it follows that Newton's method converges to 1 precisely if $0 < x_0 < 2$, since $x_0 = 0$ yields $x_1 = 2$, and F is concave and monotonically decreasing to $-\infty$ on $[0, 2)$. Any $x_0 > 2$, and therefore also any $x_0 < 0$, produces an iteration diverging to ∞.

■

Problem 74 *The bisection method is popular because it is robust: it will always work subject to minimal constraints. However, it is slow: if the Secant works, then it converges much more quickly. How can we combine these two algorithms to get a fast, robust method? Consider the following problem: Solve*

$$f(x) = 1 - \frac{2}{x^2 - 2x + 2}$$

on $[-10, 1]$. You should find that the bisection method works (slowly) for this problem, but the Secant method will fail. So write a hybrid algorithm that switches between the bisection method and the secant method as appropriate. Take care to document your code carefully, to show which algorithm is used when. How many iterations are required?

Appendix A

The First Appendix

The appendix fragment is used only once. Subsequent appendices can be created using the Chapter Section/Body Tag.

Afterword

The back matter often includes one or more of an index, an afterword, acknowledgements, a bibliography, a colophon, or any other similar item. In the back matter, chapters do not produce a chapter number, but they are entered in the table of contents. If you are not using anything in the back matter, you can delete the back matter TeX field and everything that follows it.